SPECIAL REPORT 94-19

CRREL

CALGYP: A Simulation Model for Calcite and Gypsum Precipitation–Dissolution in Soils

Giles M. Marion

July 1994

Abstract

This report documents the CALGYP model which is designed to simulate calcite and gypsum precipitation–dissolution in soils. CALGYP is a process model that is easy to parameterize, and is designed for long-term simulations (> 1000 years). The CALGYP model has five components: soil parameterization, chemical thermodynamic relations, deterministic and stochastic rainfall models, an evapotranspiration model, and subroutines that calculate water, calcium, and sulfate fluxes through the soil. The stochastic rainfall model is based on probability distributions for interarrival times (days between rainfall events) and rainfall amounts and is designed to simulate the long-term mean annual rainfall and variability in annual rainfall for specific sites. The model is currently parameterized for seven climatic sites in the desert Southwest. However, climate (temperature and rainfall) can be altered and other minerals included, which makes the CALGYP model potentially applicable across a wider range of environmental conditions including freezing–thawing systems. A separate program, Rainmodule, is included to facilitate inclusion of new sites and to alter rainfall patterns for current sites. Instructions for utilization and a FORTRAN-77 source code listing are included with the report.

For conversion of SI metric units to U.S./British customary units of measurement consult ASTM Standard E380-89a, *Standard Practice for Use of the International System of Units,* published by the American Society for Testing and Materials, 1916 Race St., Philadelphia, Pa. 19103.

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U.S. Army Corps of Engineers
Cold Regions Research & Engineering Laboratory

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Giles M. Marion

July 1994

Prepared for
OFFICE OF THE CHIEF OF ENGINEERS

PREFACE

This report was prepared by Dr. Giles M. Marion, Research Physical Scientist, of the Geochemical Sciences Branch, Research Division, U.S. Army Cold Regions Research and Engineering Laboratory. Funding was provided by DA Project 4A161102AT24, *Research in Snow, Ice and Frozen Ground,* Tasks EC and SC, Work Units B03, *Soil Solute Interactions at Low Temperature,* and F02, *Chemical Processes in Frozen Soil.*

The author thanks Andrew Sezak for assistance in translating the CALGYP program to FORTRAN and Dr. C.M. Reynolds and Dr. S.A. Grant for technically reviewing earlier drafts of this report.

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CALGYP: A Simulation Model for Calcite and Gypsum Precipitation–Dissolution in Soils

GILES M. MARION

INTRODUCTION

Calcite ($CaCO_3$) and gypsum ($CaSO_4 \cdot 2H_2O$) are common secondary minerals precipitating in both hot-dry and cold-dry soils (Tedrow 1977, Harden et al. 1991, Marion et al. 1993). Soil solution pH in calcareous soils is largely controlled by the solubility of calcite. Quantifying the chemical behavior of semi-arid to arid soils in both hot and cold regions requires explicit recognition of calcite and, to a lesser extent, gypsum. The CALGYP model was originally developed to predict calcite and gypsum formation in desert soils of the Southwest. However, climates can be altered and other minerals included in the model, which makes the CALGYP model potentially applicable across a wider range of environmental conditions. For example, CALGYP could be used to assess the long-term consequences of hazardous waste stabilization in a $CaCO_3$ matrix (a process currently under review at CRREL) where the net effect over time is a gradual dissolution and removal of $CaCO_3$. Or CALGYP could be used to simulate salt movement through cold regions soils such as those that exist along the Tanana River of interior Alaska, which are frequently saturated with respect to both calcite and gypsum (Marion et al. 1993).

Since the first paper based on this model (then called CALDEP) was published (Marion et al. 1985), copies of the computer code have been given to interested scientists. But until now, this model has not been documented in a publication that would render the model more readily available to interested scientists. The objective of this report is to document CALGYP, explaining the theoretical background, the practical use, the limitations of the model, and how to alter the model for new sites. Also included are the FORTRAN source code listing; a copy of the FORTRAN program on disk is available from the author on request.

MODEL STRUCTURE

Three principles guided the development of the CALGYP model.

1. The model must be process-based. Only at the process level can we understand fundamentally how soil processes and properties interact to control soil development.
2. Model parameters must be easily estimated. This would facilitate its application to other sites.
3. The model must be appropriate for long-term simulations (> 1000 years). This latter principle requires simplification to improve computational time.

The CALGYP model has five components: soil parameterization, chemical thermodynamic relations, stochastic and deterministic rainfall models, an evapotranspiration model, and subroutines which calculate water, calcium, and sulfate fluxes through the soil.

Soil parameterization

CALGYP is a compartment model that can be parameterized to contain 1 to 10 layers (Fig. 1). Model inputs for each layer include layer thickness, bulk density, water contents initally and at soil water matric suctions of 0.01 MPa (field capacity) and 1.5 MPa (permanent wilting point), initial soil calcite and gypsum contents, initial concentrations of soluble Ca and SO_4-S, and initial soil pH.

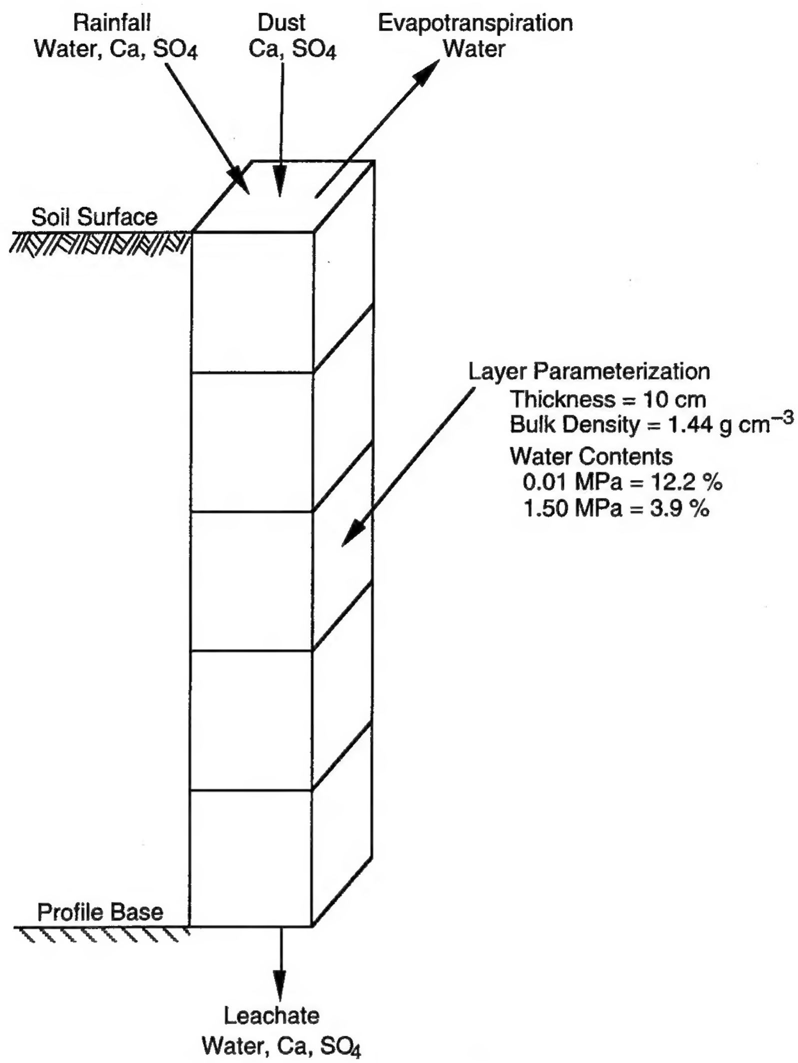

Figure 1. Schematic diagram of the CALGYP model.

A model for soil CO_2, developed from a study near Tucson, Arizona (Parada et al. 1983), allows CO_2 concentration to vary spatially and seasonally (Marion et al. 1985). Atmospheric inputs include the Ca and SO_4-S content of rainfall and dust.

Chemical thermodynamic relations

The chemical equilibrium equations used in this model include the following:

$$(CO_2)/P_{CO2} = K_1 \quad (1)$$

$$pK_1 = 1.14 + 0.0131\,t \quad (2)$$

$$(H^+)(HCO_3^-)/(H_2O)(CO_2) = K_2 \quad (3)$$

$$pK_2 = 6.54 - 0.0071\,t \quad (4)$$

$$(H^+)(CO_3^{2-})/(HCO_3^-) = K_3 \quad (5)$$

$$pK_3 = 10.59 – 0.0102\,t \quad (6)$$

$$(Ca^{2+})(CO_3^{2-}) = K_4 \quad (7)$$

$$pK_4 = 7.95 + 0.0125\,t \quad (8)$$

$$(Ca^{2+})(SO_4^{2-})(H_2O)^2 = K_5 \quad (9)$$

$$pK_5 = 4.62 + 0.0006\,t \quad (10)$$

$$(Ca^{2+})(SO_4^{2-})/(CaSO_4^o) = K_6 \quad (11)$$

$$pK_6 = 2.23 + 0.0019\,t \quad (12)$$

where pK is the negative logarithm of the equilib-

rium constant, t is temperature (°C), and parentheses refer to activities. The equilibrium constants and their temperature dependencies were estimated from equilibrium data over the temperature range, 0 to 40 °C (Garrels and Christ 1965). The intercept term in eq 8 was selected to yield a pK of 8.26 at 25 °C, which was the mean of several B_{k2} horizon samples from the desert LTER site equilibrated at 25 °C under a fixed CO_2 concentration (500 ppm) for 10 days (Marion et al. 1990).

Single-ion activities (a) of ions having aqueous solution concentrations of c are estimated by

$$a = \gamma c \tag{13}$$

where γ is the single-ion activity coefficient, which was estimated with the Davies equation (Davies 1962)

$$\log \gamma = - A z^2 [\sqrt{I}/(1.0 + \sqrt{I}) - 0.3 I] \tag{14}$$

where z is the ionic valence, I is the ionic strength which is defined as

$$I = 0.5 \Sigma (c_i z_i^2) \tag{15}$$

and A is the Debye-Hückel constant which is given by

$$A = 0.4918 + 6.6098 \times 10^{-4} t + 5.0231 \times 10^{-6} t^2 \tag{16}$$

over the temperature range: 0–40 °C (Robinson and Stokes 1965).

Critical to the performance of these models is the mechanism for estimating soil solution pH, because of the strong influence of pH on $CaCO_3$ solubility. For a pure $CaCO_3$–$CaSO_4$ solution in the pH range of 7–8.5, the following charge balance holds:

$$2[Ca^{2+}] = [HCO_3^-] + 2[CO_3^{2-}] + 2[SO_4^{2-}] \tag{17}$$

where brackets refer to concentrations. For a system in equilibrium with solid $CaCO_3$, this equation can be rewritten as:

$$\frac{2K_4 (H^+)^2}{\gamma_{Ca} K_3 K_2 K_1 P_{CO2}} = \frac{K_1 K_2 P_{CO2}}{(H^+) \gamma_{HCO3}} + \frac{2K_1 K_2 K_3 P_{CO2}}{(H^+)^2 \gamma_{CO3}} + 2 [SO_4^{2-}] . \tag{18}$$

Given the P_{CO2} (partial pressure of CO_2) and the SO_4-S concentration, eq 18 is solved for (H^+), which is then used to control $CaCO_3$ solubility.

For a system in equilibrium with both solid calcite and gypsum, the sulfate term in brackets (eq 17 and 18) may be replaced by

$$\frac{K_5 K_1 K_2 K_3 P_{CO2}}{K_4 \gamma_{SO4} (H^+)^2} \tag{19}$$

Compared to equilibrium with pure calcite, simultaneous equilibrium of gypsum and calcite significantly depresses the equilibrium pH and increases the equilibrium Ca concentrations (Fig. 2). In the CALGYP model, eq 18 is used to estimate solution pH (after $CaCO_3$ begins to precipitate), so that soil

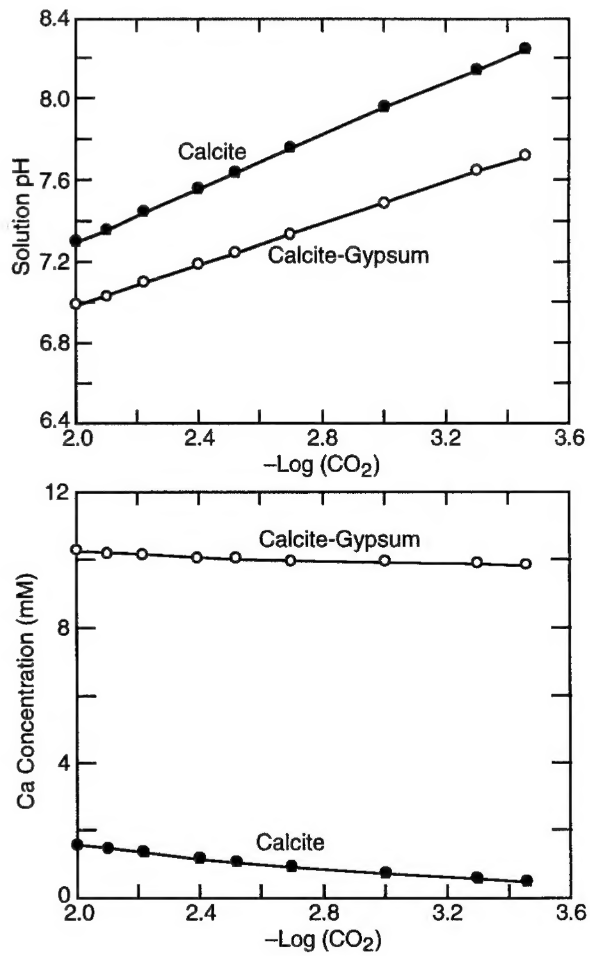

Figure 2. Theoretical (A) pH and (B) Ca concentrations for pure calcite and calcite-gypsum solutions as functions of the partial pressure of carbon dioxide at 25 °C.

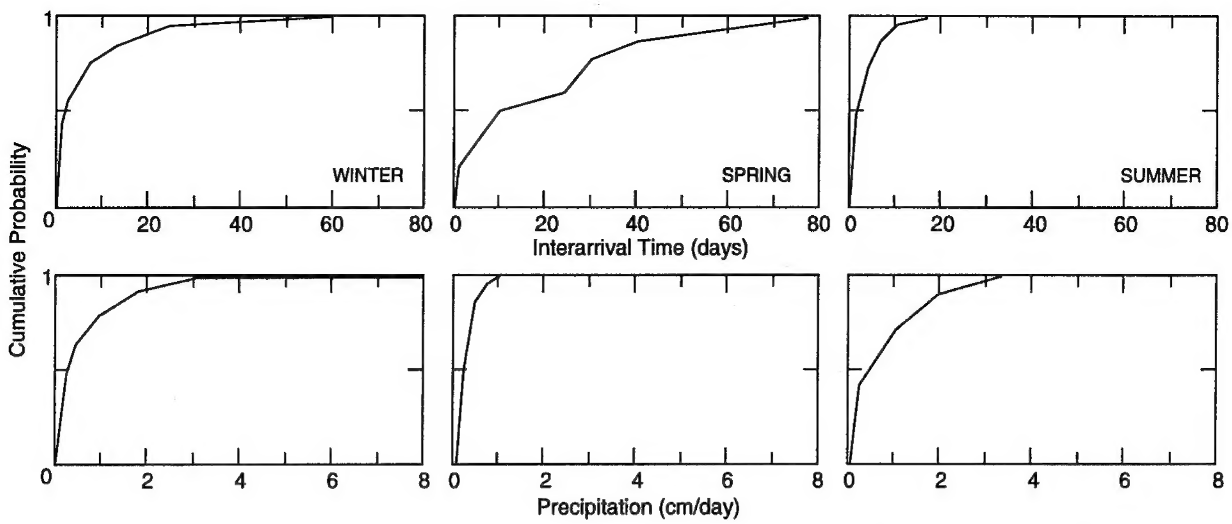

Figure 3. Cumulative probabilities for interarrival days and daily rainfall for the Tucson site.

solution pH is a continuous function of soil solution sulfate concentration. Empirical justification for this assumption was demonstrated in a previous paper (Marion and Schlesinger in press).

If soil solution sulfate concentrations are "zero," CALGYP will by-pass the sulfate equilibrium routines and will calculate chemical equilibrium for a pure calcite system. One can also effectively bypass calcite equilibrium and its pH dependence (eq 18) by assigning the initial soil an arbitrarily low pH of 5.0. At this low pH, it is doubtful that Ca concentrations will ever build up to the point where calcite would precipitate given normal soil CO_2 concentrations.

Rainfall models

The stochastic rainfall model controls input of water and is based on probability distributions for interarrival times (the number of days between rainfall events) and the rainfall amounts for specific seasons at specific sites (Fig. 3). Sites currently in the model include Yuma, Phoenix, and Tucson in Arizona; Albuquerque, Roswell, and Clayton in New Mexico; and El Paso, Texas. A random-number generator is used to select the interarrival times and rainfall amounts for each year from the cumulative probability distributions. This stochastic model is designed to reproduce the long-term average annual rainfall and the variability in annual rainfall for a specific site (Marion et al. 1985).

In addition to the stochastic rainfall model, CALGYP also includes an option for a deterministic rainfall model that allows the user to specify the yearly rain dates and rainfall amounts for a specific site. The same rainfall pattern is then used year-after-year.

Evapotranspiration model

The evapotranspiration model, which is primarily a function of temperature, controls the loss of water and consists of three steps. First, potential evapotranspiration is calculated using Thornthwaite's equation (Thornthwaite 1948, Marion et al. 1985). Second, Thornthwaite's potential evapotranspiration is converted to pan evaporation using a derived, empirical relationship with temperature for Southwestern deserts (Fig. 4). And third, actual evapotranspiration is calculated as a function of soil moisture and pan evaporation between field capacity (0.01 MPa) and permanent wilting point (1.5 MPa) (Fig. 5). Calibration of the third step is based on field measurements from a *Larrea tridentata* (creosote bush) site at the Jornada Desert Long-Term Ecological Research site near Las Cruces, New Mexico (Marion et al. 1985). Water loss is assumed to occur at the potential rate (ratio = 1.00) in the upper 45.4 % of the available moisture range; in the lower 54.6 % of the range, water loss is a linear function of soil moisture (Fig. 5).

CALGYP includes options to change the climatic variables of rainfall and temperature. For a temperature change for the Southwestern desert sites, CALGYP assumes that monthly pan evaporation is decreased (increased) by an amount proportional to the mean annual temperature decrease (increase) (Fig. 6). For a fuller discussion on altering climate within and outside the desert

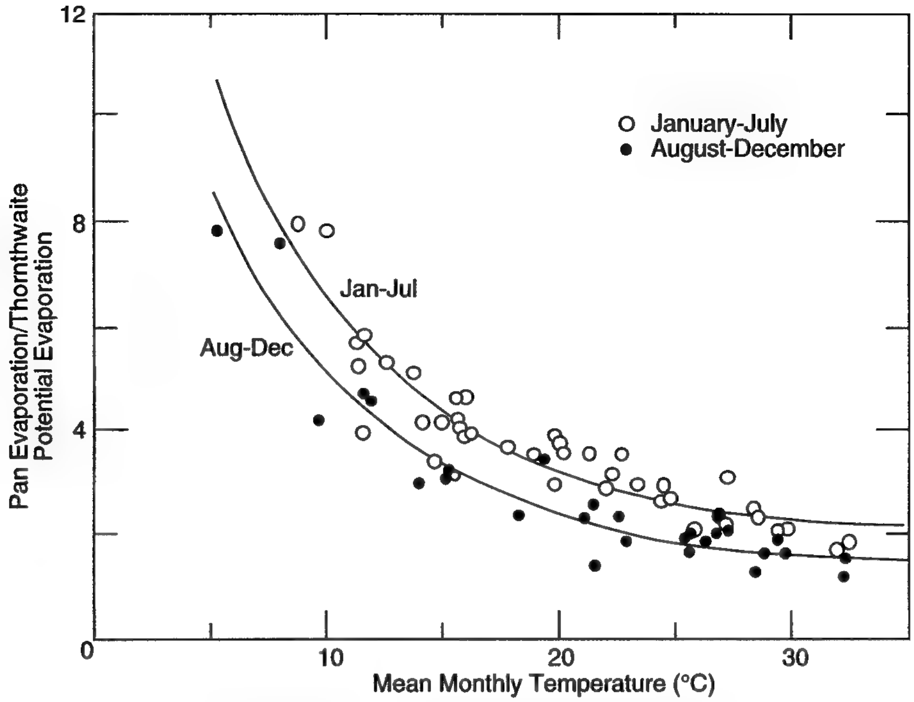

Figure 4. Pan evaporation/Thornthwaite potential evapotranspiration ratio as a function of mean monthly temperature for Southwestern desert sites.

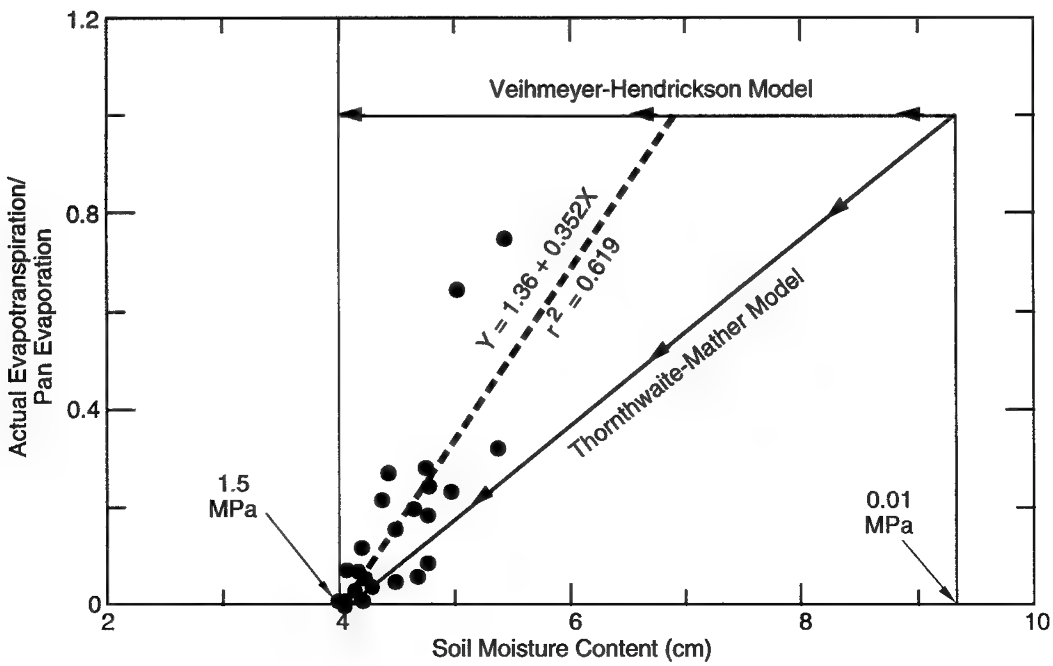

Figure 5. Relationship of the actual evapotranspiration/pan evaporation ratio as a function of soil moisture content.

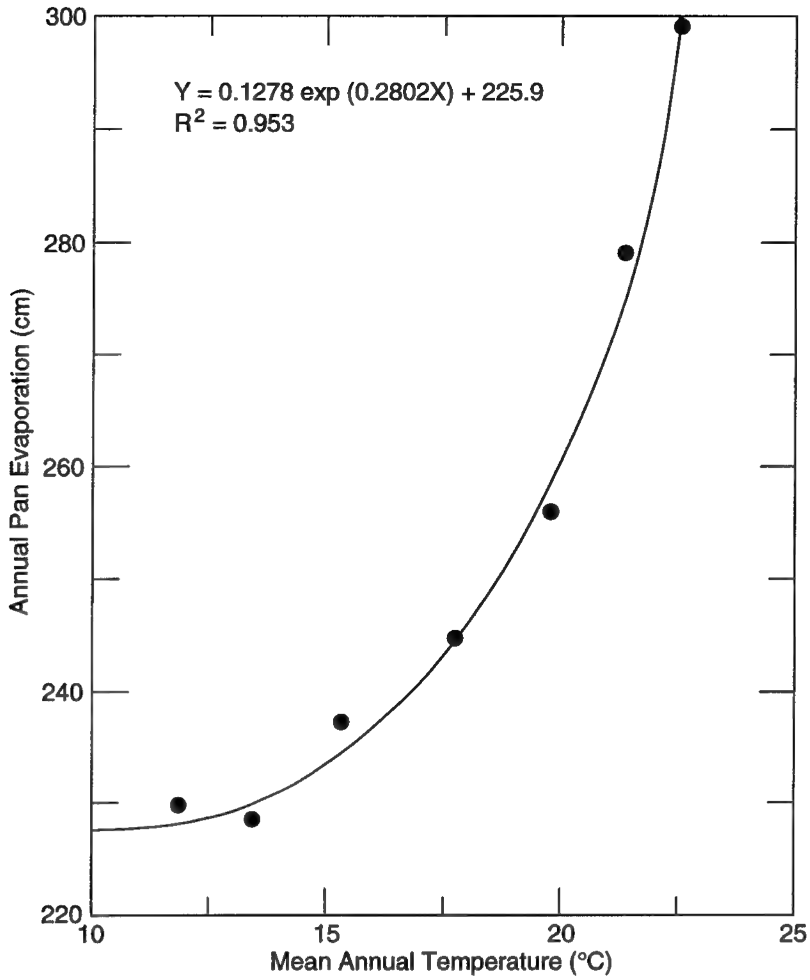

Figure 6. Annual pan evaporation (calculated) as a function of mean annual temperature.

Southwest, see *Altered Climate and Chemistry.*

Water and solute flux

A daily time-step is used to assess the fluxes of water and solutes through the soil. All rainfall is assumed to enter the uppermost soil layer (Fig. 1); the model ignores vegetative interception of rainfall and surface runoff. Only saturated flow of water is considered in these models. If the water-holding capacity of a layer is exceeded (i.e., water content > field capacity), excess water moves into progressively deeper layers. Water flux beyond the base of the soil profile is treated as leachate and is assumed lost from the system. Solutes are assumed to move with the mass flow of water. Water that enters a given layer is mixed with the pre-existing water and solutes are equilibrated chemically with the solid and gas phases. Therefore, the excess water that passes through a given layer contains an equilibrated concentration of solutes before passing to the deeper layers. During drying cycles, water is first extracted from the surface layer and then from progressively deeper layers using the evapotranspiration model previously mentioned.

CALGYP FLOWCHART

After initialization of soil properties and calculation of monthly potential evaporation, CALGYP cycles along three time steps (Fig. 7). Water loss is calculated on a daily time step. Whenever a rain event occurs, CALGYP cycles through chemical equilibrium and water flux routines to calculate the fluxes of water and solutes through the soil

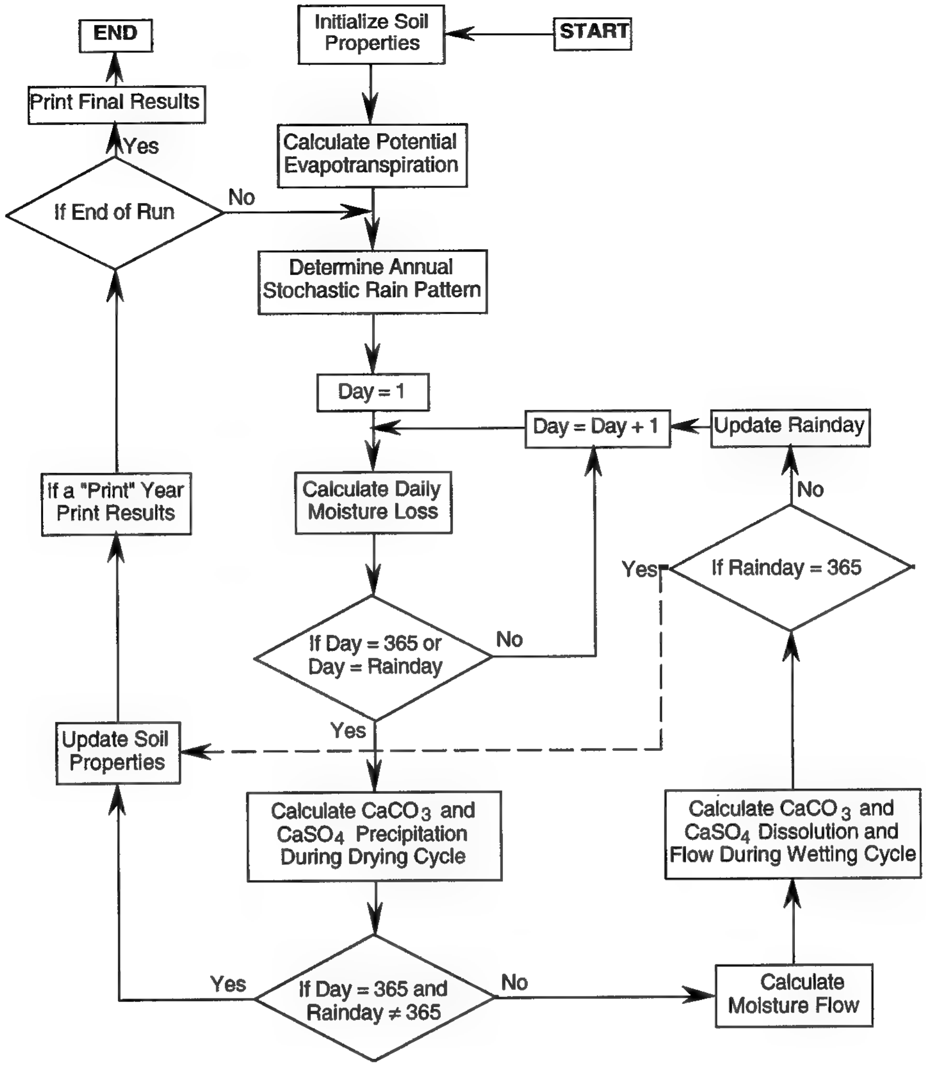

Figure 7. CALGYP program flowchart.

profile. The chemical equilibrium routines are addressed twice for each rain event. First, calcite and gypsum precipitation are calculated over the previous drying cycle up to the rain event day. Then, dissolution and flow of calcite and gypsum are calculated after the water flux determination. An annual cycle includes calculation of the stochastic rain pattern, the daily and rain event cycles, and print statements.

THE FORTRAN PROGRAM

The original version of the CALGYP program was called CALDEP because it dealt exclusively with *cal*cite *dep*osition and was written in HP Basic (Marion et al. 1985). This version required about 45 seconds of computer time to simulate a year of soil development on an HP 9816 microcomputer. This program was translated into a TrueBASIC version for operation on an Apple Macintosh IIcx computer. When *gyp*sum was added to the model, the name was changed to CALGYP. The CALGYP program required 11 to 22 seconds/year on 16-MHz and 25-MHz Apple Macintosh computers, respectively. Recently CALGYP was translated to FORTRAN, primarily to increase portability to other computer systems and to improve computational time. The present FORTRAN version requires 0.22 seconds/year running on a 33-MHz Apple Macintosh Quadra 800 using the MacFortran II compiler optimized for the Motorola 68040 processor (Absoft 1993). To simulate 10,000 years of change now requires 37 minutes with the FOR-

TRAN version on a fast microcomputer compared to 5.2 days with the original HP Basic version on a slower microcomputer. This 200-fold improvement in computational speed is a major enhancement because this program must be able to simulate slow change over very long periods.

A major effort was made to adhere to the FORTRAN 77 ANSI Standard in the translation. For example, CALGYP uses an 80-column statement line where columns 1–5 are statement labels, column 6 is a continuation column, columns 7–72 are used for statements, and columns 73–80 are used for commentary. To facilitate the translation, variable names were retained between programs except to shorten names with > six characters in the TrueBASIC version to ≤ six characters in the FORTRAN version. FORTRAN assumes, unless otherwise declared, that variables beginning with the letters "I, J, K, L, M, and N" are integer variables and all other initial letters refer to real variables. In order to retain the same variable names between programs, this restriction required formal declaration of some real and integer variables in the FORTRAN version. Also, in a few cases, integer arithmetic had to be rewritten in terms of real variables to preserve meaning between programs.

The CALGYP program consists of a main program, also called *CALGYP*, and eight subroutines, four for climate and four for chemical equilibrium. In addition, a separate program called Rainmodule is included in order to facilitate altering rainfall patterns. CALGYP and Rainmodule use one external library routine called "rand" (UNIX library) which selects random numbers between 0.0 and 1.0. Program listings are included in Appendices A and B.

In contrast to the "modular" approach where the main program primarily "calls" other subprograms (Nyhoff and Leestma 1985, Plummer et al. 1988), the *CALGYP* main program directly performs many important tasks. *CALGYP:* 1) controls screen queries, 2) contains the bulk of the data used by the program, 3) initiates variables, 4) calculates moisture flow, 5) mixes solutions, 6) updates soil properties, and 7) prints results.

The four climate subroutines are *Detrain*, *Raindate*, *Rainfall*, and *Seasons*. *Detrain* allows the user to specify rain dates and rainfall amounts for a given year at a specific site. This yearly pattern is then reused year after year (the "deterministic" rain model). The subroutines *Raindate*, *Rainfall*, and *Seasons* are used to develop the "stochastic" rain model, which varies rain dates and rainfall amounts over annual cycles based on probability distributions and a random-number generator. *Raindate* and *Rainfall* calculate the annual rain dates and rainfall amounts for a specific site, respectively. *Seasons* calculates the proper season (e.g., winter, spring, summer) for a given day of the year and site. This controls the proper probability distributions used in the *Raindate* and *Rainfall* subroutines.

The four chemical subroutines are *Constants*, *Ion*, *Hact*, and *Equil*. *Constants* calculates the equilibrium constants (eq 1–12) and the Debye-Hückel constant "A" (eq 14 and 16) for a specific temperature. Mean monthly air temperatures for a specific site are used for these temperature calculations. *Ion* calculates the single-ion activity coefficients of univalent and bivalent ions using the Davies equation (eq 14). *Hact* calculates the H activity using eq 18. *Equil* calculates the equilibrium composition of solutions accounting for the $CaSO_4^0$ ion-pair and the precipitation and dissolution of calcite and gypsum.

PROGRAM INPUT

CALGYP program

CALGYP input occurs primarily through screen queries, DATA statements, and two subroutines (*Detrain* and *Constants*). CALGYP is designed to work interactively with on-screen prompts requesting information and options to control the simulation (See Table 1). The information requested includes:

(1) Site Selection? This prompt requests that the user select one of seven sites by entering the site designation (Table 1), then the RETURN key.

(2) Current Climate or Altered Climate? Enter proper designation, then RETURN. If Altered Climate is selected, then:

(a) Change in temperature (°C). Enter temperature change (+ for increase, – for decrease).

(b) Fractional change in rainfall amount during drier climate. If rainfall is to decrease 10%, enter 0.10, then RETURN. Wetter climates require altering the probability distributions (See *Altered Climate and Chemistry*).

(3) Title? Enter any alphanumeric title up to 50 characters, then RETURN.

(4) Number of Soil Horizons? CALGYP can work with 1 to 10 horizons (layers). This

Table 1. An example of the CALGYP screen query input.

```
Select Site:
   1 = El Paso, TX (21.6cm)
   2 = Albuq., NM (21.1cm)
   3 = Clayton, NM (37.8cm)
   4 = Roswell, NM (31.6cm)
   5 = Yuma, AZ (8.5cm)
   6 = Phoenix, AZ (18.9cm)
   7 = Tucson, AZ (28.4cm)
7
Climate Option? Current Climate = 1, Altered Climate = 2
2
Enter Delta Temperature=(°C,default=0.0,no change)
-5
Enter Fractional Change in Rainfall Amount during
      Drier Climate = (default = 0.0, no change)
0.1
Title?
TUCSON SIMULATION OF ALTERED CLIMATE
Number of Soil Horizons (Max=10)?
10
Years to Simulate?
1
Print Interval?
1
Deterministic (1) or Stochastic (2) Rainfall Model?
2
Seed for Random Number Generator?
123
```

number must not exceed the dimension of the soil horizon properties specified in the DATA statements.

(5) Years to Simulate? Enter the number of years that you wish this simulation to run, then RETURN.

(6) Print Interval? At what yearly interval do you wish intermediate results printed. For example, for a 1000-year simulation, you may wish to print profile descriptions at 200-year intervals.

(7) Deterministic or Stochastic Rainfall Model? Enter designation for appropriate rainfall model. If stochastic is selected, then:

(a) Seed for Random Number Generator? Enter integer of 1-5 digits. Using the same Seed in runs will produce the same sequence of random numbers, which is particularly useful during the development and debugging stages.

Table 1 is an example of a screen query that selects the Tucson site with altered climate (5 °C colder with 10% less rainfall). The number of soil horizons is 10, and the simulation runs for one year with a printout at one year. The stochastic rainfall model was selected with a Seed of 123 for the random number generator.

Most of the data used to parameterize the model are stored in DATA statements within the CALGYP program. These DATA statements start on p. 2 of the program listing (App. A). To make changes in these data requires entering and altering the source code.

The first DATA statement lists the mean monthly air temperatures (°C) for the seven sites. Commentary in columns 73-80 identifies the specific site. The temperature data are followed by several DATA statements that specify the parameters for the stochastic rainfall model by site and season. Five of the sites have two rainfall seasons (winter and summer). Phoenix and Tucson have three rainfall seasons (winter, spring, summer). Details on the derivation of these distributions were discussed in Marion et al. (1985). The variables D(I,J,K) and R(I,J,K) are probabilities and corresponding daily rainfall amounts. For example, the probability is 0.837 of a daily rainfall amount ≤ 1.00 cm for El Paso in the winter (App. A). For this site and season, a random number of 0.600 would fall between rainfall amounts of 0.25 and 0.50 cm; linearly interpolating gives 0.29 cm of rain at a probability of 0.600. In a few cases, dummy probabilities (> 1.00) are present in order to complete matrices. The only physically meaningful probabilities are ≤ 1.00. For example, the only meaningful probabilities [D(I,J,K)] for Phoenix in the spring are 0.000 to 1.000; the values ranging from 1.1 to 1.6 are dummy variables as are the corresponding

rainfall amounts ranging from 1.25 to 3.07 cm. The variables Freq (I,J,K) and Inter (I,J,K) are the probabilities and corresponding interarrival days (the number of days between rainfall events). For El Paso in the winter, the probability is 0.765 of ≤ 10 days between rain events. For this site and season, a random number of 0.600 corresponds to an interarrival time of 5.8 days.

Subsequent DATA statements define the basic soil properties of the system. Properties that must be specified by horizon include thickness, bulk density, soil water concentrations at 0.01 MPa (field capacity), 1.5 MPa (permanent wilting point), and at first, initial $CaCO_3$ and soluble Ca, initial soil solution H activity and soil atmospheric CO_2 concentration, and initial $CaSO_4$ and soluble SO_4. The program allows the user to change monthly CO_2 concentrations in the soil profile by using a single monthly multiplier for the entire profile. In the present program (App. A), the winter months' (November–February) CO_2 concentrations are increased by 58.8% during the other months (Marion et al. 1985).

The final data statements define the atmospheric properties that include the dust Ca and SO_4 contents and the rain Ca and SO_4 concentrations. CALGYP only considers precipitation and dissolution of calcite and gypsum. Other minerals that might contribute to Ca and SO_4 input are ignored, which is a reasonable assumption for Southwestern desert soils because of the generally low rates of mineral weathering (Gile et al. 1981, Machette 1985, Harden et al. 1991, McFadden et al. 1991). If weathering of minerals other than calcite and gypsum were important and these rates were known, they could be included with dust inputs.

The subroutine *Detrain* contains the rain dates and rainfall amounts for the deterministic rain model. This subroutine requires specification of the rain dates (Julian day) and rainfall amounts (cm) in the appropriate DATA statements (*Raindy* and *Raina*). Also, the *Dimension* statement and the variable, *Sumfre,* must be changed to reflect the total number of rain events/year. *Constants* contains the chemical thermodynamic constants and their temperature dependence.

Rainmodule Program

The Rainmodule program was designed to facilitate inclusion of new sites with new rainfall patterns and for altering rainfall for current sites. The structure of this program is similar to that used for the stochastic model in *CALGYP*. Running this model "as is" will result in rainfall patterns identical to those used in *CALGYP*. By trial and error, one can alter either the frequency distributions or the variables "Newj" or "Numb" to increase or decrease rain dates or rainfall amounts. In general, the frequency distributions are derived from short-term records (e.g., 3–10 years) which may be wetter or drier than normal. The variables Newj and Numb are used to increase or decrease the number of rain dates per year, respectively, in order to match the long-term (40–100 year climate record) mean annual rainfall for a specific site. Newj adds rain dates increasing rainfall; Numb assigns 0.0 to rainfall amounts, effectively eliminating dates and decreasing rainfall. Manipulation of the frequency distributions will be discussed under *Altered Climate and Chemistry*.

PROGRAM OUTPUT

CALGYP program

Output from CALGYP is printed to a file called "CaData" in three major blocks. Table 2 contains an example for a 1000-year simulation with intermediate results printed at 200-year intervals.

The first block contains the title and a few key run options followed by a climate summary (monthly temperatures and calculated potential evapotranspiration), the initial soil profile, and atmospheric chemical drivers.

The second block, repeated several times, contains intermediate soil profile properties at the "Print" interval. These properties include $CaCO_3$ and $CaSO_4$ contents, the bulk density (which increases as mineral salts precipitate), the total amount of water, Ca, and S leached past the base of the soil profile through the specified year, and the annual rainfall and evapotranspiration for the specified year.

The third block includes a few additional soil profile properties at the end of the simulation, such as moisture content, H ion activity, and soluble Ca and SO_4. Also total rain and total evapotranspiration for the entire simulation are printed. And finally residual dust Ca and SO_4 are printed. The model accumulates dust at the soil surface on a daily basis and washes it into the profile whenever it rains. "Residual dust" refers to the amount of Ca and SO_4 that has accumulated as dust at the soil surface between the last rain and the end of the year for the last year of the simulation. This final data block may be useful intrinsically (e.g., for mass balance calculations) as well as for providing

Table 2. Sample output of the CALGYP model for a 1000-year simulation for the Tucson site.

```
4/18/94 10:37                Macintosh HD:MPW:CaData

TUCSON 1000 YR SIMULATION
SITE =   7
Stochastic Rainfall Model with Seed =  123

    CLIMATIC SUMMARY
         Month     Temp(C)   Pot.Evap.(g/cm2)
           1        10.2          10.90
           2        11.8          11.77
           3        14.3          16.26
           4        18.1          20.44
           5        22.6          27.47
           6        27.8          35.39
           7        30.0          41.19
           8        28.9          28.19
           9        26.7          24.37
          10        20.8          18.54
          11        14.6          12.34
          12        10.8           9.09

INITIAL SOIL PROFILE
Hori Thick  BD       CO2          H          CaCO3        Ca         CaSO4        SO4
      cm   g/cm3     atm                    gCa/cm2     gCa/cm2      gS/cm2      gS/cm2
  1  10.0  1.44  0.379E-03  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04
  2  10.0  1.44  0.687E-03  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04
  3  10.0  1.44  0.976E-03  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04
  4  10.0  1.44  0.128E-02  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04
  5  10.0  1.44  0.160E-02  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04
  6  10.0  1.44  0.191E-02  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04
  7  10.0  1.44  0.214E-02  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04
  8  10.0  1.44  0.227E-02  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04
  9  10.0  1.44  0.241E-02  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04
 10  10.0  1.44  0.254E-02  0.100E-07  0.000E+00  0.864E-05  0.000E+00  0.144E-04

ATMOSPHERIC CHEMICAL CONDITIONS
Dustca(gCa/cm2/yr)  Precca(mgCa/l)  Dusts(gS/cm2/yr)  Precs(mgS/l)
    0.8614E-04           .00            0.7993E-05          .00

----------------------------------------------------------------------------------

YEAR =  200

CACO3(gCa/cm2) = 0.00000E+00 0.16325E-04 0.13443E-03 0.55263E-02 0.42430E-02
CACO3(gCa/cm2) = 0.24938E-02 0.13452E-02 0.45815E-03 0.23268E-03 0.17588E-03

CASO4(gS/cm2) = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
CASO4(gS/cm2) = 0.00000E+00 0.00000E+00 0.60269E-04 0.19028E-03 0.30192E-03

Bulk Density(g/cm3) =  1.4400  1.4400  1.4400  1.4414  1.4411
Bulk Density(g/cm3) =  1.4406  1.4403  1.4401  1.4402  1.4402

Leach(cm) = 0.6681E+01  Leacca(gCa/cm2) =0.47531E-03  Leachs(gS/cm2) =0.17596E-03

Annual Rain(cm) = 27.899     Annual Evap(cm) = 27.858

----------------------------------------------------------------------------------

YEAR =  400

CACO3(gCa/cm2) = 0.00000E+00 0.63449E-04 0.65553E-03 0.10642E-01 0.89438E-02
CACO3(gCa/cm2) = 0.52801E-02 0.28194E-02 0.94581E-03 0.34664E-03 0.17595E-03

CASO4(gS/cm2) = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
CASO4(gS/cm2) = 0.00000E+00 0.00000E+00 0.38755E-03 0.12687E-02 0.30205E-03
```

Table 2 (Cont'd). Sample output of the CALGYP model for a 1000-year simulation for the Tucson site.

```
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Bulk Density(g/cm3) =  1.4400  1.4400  1.4402  1.4427  1.4422
Bulk Density(g/cm3) =  1.4413  1.4407  1.4404  1.4408  1.4402

Leach(cm) = 0.6681E+01  Leacca(gCa/cm2) =0.47531E-03  Leachs(gS/cm2) =0.17596E-03

Annual Rain(cm) = 29.237     Annual Evap(cm) = 30.964

-----------------------------------------------------------------------------------

YEAR =  600

CACO3(gCa/cm2) = 0.13084E-04 0.39974E-04 0.59466E-03 0.17612E-01 0.13134E-01
CACO3(gCa/cm2) = 0.78798E-02 0.39994E-02 0.12391E-02 0.40816E-03 0.18832E-03

CASO4(gS/cm2) = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
CASO4(gS/cm2) = 0.00000E+00 0.19832E-03 0.93836E-03 0.19800E-02 0.45282E-03

Bulk Density(g/cm3) =  1.4400  1.4400  1.4401  1.4444  1.4433
Bulk Density(g/cm3) =  1.4420  1.4411  1.4408  1.4412  1.4403

Leach(cm) = 0.6681E+01  Leacca(gCa/cm2) =0.47531E-03  Leachs(gS/cm2) =0.17596E-03

Annual Rain(cm) = 21.983     Annual Evap(cm) = 21.989

-----------------------------------------------------------------------------------

YEAR =  800

CACO3(gCa/cm2) = 0.40850E-05 0.56173E-04 0.20961E-03 0.24291E-01 0.17550E-01
CACO3(gCa/cm2) = 0.10510E-01 0.53865E-02 0.16162E-02 0.49783E-03 0.21882E-03

CASO4(gS/cm2) = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
CASO4(gS/cm2) = 0.00000E+00 0.51036E-03 0.85479E-03 0.29788E-02 0.79254E-03

Bulk Density(g/cm3) =  1.4400  1.4400  1.4401  1.4461  1.4444
Bulk Density(g/cm3) =  1.4426  1.4416  1.4409  1.4417  1.4405

Leach(cm) = 0.6681E+01  Leacca(gCa/cm2) =0.47531E-03  Leachs(gS/cm2) =0.17596E-03

Annual Rain(cm) = 30.808     Annual Evap(cm) = 30.486

-----------------------------------------------------------------------------------

YEAR =  1000

CACO3(gCa/cm2) = 0.00000E+00 0.69365E-04 0.30493E-03 0.30038E-01 0.22281E-01
CACO3(gCa/cm2) = 0.13423E-01 0.65728E-02 0.20215E-02 0.59955E-03 0.22829E-03

CASO4(gS/cm2) = 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
CASO4(gS/cm2) = 0.00000E+00 0.20971E-03 0.12965E-02 0.42528E-02 0.92806E-03

Bulk Density(g/cm3) =  1.4400  1.4400  1.4401  1.4475  1.4456
Bulk Density(g/cm3) =  1.4434  1.4418  1.4412  1.4424  1.4406

Leach(cm) = 0.6681E+01  Leacca(gCa/cm2) =0.47531E-03  Leachs(gS/cm2) =0.17596E-03

Annual Rain(cm) = 31.399     Annual Evap(cm) = 29.940

-----------------------------------------------------------------------------------

FINAL SOIL PROFILE CONCENTRATIONS
 See last year above for other final soil properties
```

Table 2 (Cont'd).

```
4/18/94 10:37                Macintosh HD:MPW:CaData

Hori   Moisco(g/cm2)    H activity     Ca(gCa/cm2)    SO4(gS/cm2)
  1     0.81111E+00     0.71021E-08    0.15696E-04    0.14565E-05
  2     0.89038E+00     0.67547E-08    0.43346E-04    0.64568E-05
  3     0.14261E+01     0.89597E-08    0.91333E-04    0.24335E-04
  4     0.67716E+00     0.12201E-07    0.69966E-04    0.33322E-04
  5     0.56160E+00     0.15032E-07    0.76210E-04    0.41713E-04
  6     0.56160E+00     0.23877E-07    0.23684E-03    0.17419E-03
  7     0.56160E+00     0.28090E-07    0.32912E-03    0.24847E-03
  8     0.56160E+00     0.28948E-07    0.32946E-03    0.24831E-03
  9     0.56160E+00     0.29846E-07    0.32981E-03    0.24814E-03
 10     0.56160E+00     0.30658E-07    0.33013E-03    0.24798E-03

Torain(cm) =      0.286059E+05      Toevap(cm) =      0.286064E+05

Residual Dust Ca(gCa/cm2) = 0.2360E-05     Residual Dust SO4(gS/cm2) = 0.2190E-06
```

data necessary to reinitialize the model for runs with new climates or other system drivers. One could, for example, simulate alternating Pleistocene and Holocene climates.

Rainmodule output

For convenience, the current version of Rainmodule prints to the computer screen. One can get a hard copy by selecting "Print Window" to sent the output to the on-line printer. Alternatively, the user could, if desired, change the program to "Write" directly to a file as was done in CALGYP.

This program prints total rainfall and total rain events for a fixed simulation of 1000 years in 100-year blocks (Table 3). The average annual rainfall should be close to the long-term mean for the site. In this particular case for Tucson, calculated average annual rainfall was 28.6 cm compared to 28.4 cm for the long-term mean (Table 3). Note that the total rainfall in 1000 years (28,605.9 cm) is identical for both CALGYP (Table 2) and Rainmodule (Table 3) because the same Seed (123) was used for the random-number generators in both programs. Using a different Seed of 1 yields 44,833 rain events for a total of 28,675.2 cm of rain in 1000 years, which is similar but not identical to the previous run with a Seed of 123 (Table 3).

PROGRAM VALIDATION

CALGYP maintains mass balances with respect to water, calcium, and sulfate. Users should verify for themselves that the model accurately maintains these balances. CALGYP prints the necessary output to make these calculations.

Water balance is given by

(Soil Water)$_{initial}$ + Rain = (Soil Water)$_{final}$ + Evapotranspiration + Leachate.

For the 1000-year simulation (Table 2), these quantities (cm of water) are

$$14.4 + 28{,}605.9 = 7.2 + 28{,}606.4 + 6.7$$
$$28{,}620.3 = 28{,}620.3.$$

For calcium, the major sink in the soil profile is $CaCO_3$ which has accumulated 7.553×10^{-2} g Ca cm^{-2} over the 1000-year simulation (Table 2). Other sinks include $CaSO_4$ (8.36×10^{-3} g Ca cm^{-2}), Δ soluble Ca* ($+1.77 \times 10^{-3}$ g Ca cm^{-2}), leachate Ca (4.8×10^{-4} g Ca cm^{-2}), and residual dust Ca (2×10^{-6} g Ca cm^{-2}). The soil profile increased in Ca content over the 1000-year simulation by 8.614×10^{-2} g Ca cm^{-2}, which is equal to the annual atmospheric input of 8.614×10^{-5} g Ca cm^{-2} year^{-1} (Table 2) for 1000 years.

For sulfate, the major sink is $CaSO_4{\cdot}2H_2O$ which has accumulated 6.687×10^{-3} g S cm^{-2} over the 1000-year simulation (Table 2). Other sinks include Δ soluble SO_4 ($+1.131 \times 10^{-3}$ g S cm^{-2}), leachate SO_4 (1.76×10^{-4} g S cm^{-2}), and residual dust SO_4 (2×10^{-7} g S cm^{-2}). The soil profile increased in SO_4 by 7.994×10^{-3} g S cm^{-2} which is equal, within roundoff error, to the annual SO_4 dust input rate of 7.993×10^{-6} g S cm^{-2} year^{-1} (Table 2) for 1000 years.

For this particular simulation, only dust chemi-

*The change (Δ) in soluble Ca between the final (1000 yr) and initial (0 yr) of the simulation.

Table 3. Sample input and output of the rain module program for a 1000-year simulation for the Tucson site.

```
Select Site:
   1 = El Paso, TX (21.6cm)
   2 = Albuq., NM (21.1cm)
   3 = Clayton, NM (37.8cm)
   4 = Roswell, NM (31.6cm)
   5 = Yuma, AZ (8.5cm)
   6 = Phoenix, AZ (18.9cm)
   7 = Tucson, AZ (28.4cm)
7
Title?
Tucson Simulation
Fractional Change in Rain for Drier Climate.
   Default = 0.00, no change.
0.0
Seed for Random Number Generator?
123
                Rain(cm)   Rain Events
 100 yrs =      3049.7       4554
 100 yrs =      2871.1       4537
 100 yrs =      2892.7       4442
 100 yrs =      2885.6       4335
 100 yrs =      2879.0       4479
 100 yrs =      2788.4       4335
 100 yrs =      2840.2       4386
 100 yrs =      2712.4       4273
 100 yrs =      2867.2       4393
 100 yrs =      2819.7       4395
1000 yrs =     28605.9      44129
```

cal inputs were specified (Table 2). When rain chemical concentrations are also specified, then

$$\text{Ca (or } SO_4\text{-S) (g cm}^{-2}) = \text{Ca (or } SO_4 - \text{S) (mg L}^{-1}) \times \text{Rain (cm)} \times 1.0 \times 10^{-6}$$

must be added to dust inputs to determine total system chemical input.

The stochastic rain model used in CALGYP accurately predicts the mean annual rainfall and the variability in this quantity for the seven Southwestern desert sites (Marion et al. 1985). The CALGYP model using current climate typically predicts a shallower depth of $CaCO_3$ deposition than is found in most Southwestern desert soils. This is not surprising because most $CaCO_3$ is believed to have formed under earlier, "wetter" Pleistocene climates (Gile et al. 1981, Marion et al. 1985, McFadden and Tinsley 1985). CALGYP is compatible with field soils if one assumes that most pedogenic $CaCO_3$ formed during a cool-wet Pleistocene climate (Marion et al. 1985). CALGYP predicts that the time required for complete plugging of soil profiles with $CaCO_3$ requires >> 10,000 years in agreement with independent evidence (Gile et al. 1981; Marion et al. 1985). CALGYP correctly predicts the deeper deposition of the more soluble mineral, gypsum, in the soil profile relative to calcite (Fig. 8). The dependence of soil pH on sulfate concentration (eq 18) was validated recently with field data from a cold dry site in Alaska and a hot dry Mojave Desert site (Marion and Schlesinger in press). Other aspects of CALGYP have been validated previously (Marion et al. 1985, Marion and Schlesinger in press).

ALTERED CLIMATE AND CHEMISTRY

Climate

CALGYP is structured to alter both temperature and rainfall for the seven Southwestern sites currently in the model. There are, however, limitations on these alterations.

Temperature largely controls output of water through the evapotranspiration process (Fig. 4 and 6). To keep temperature within the range of data used to parameterize the model, mean monthly temperatures should be between 5 and 32 °C (Fig. 4) and mean annual temperatures should be between 12 and 23 °C (Fig. 6). Any temperature alteration should ideally be limited to these ranges. However, even in the current climate model, temperatures occasionally fall below 5 °C in the winter months for Albuquerque, Clayton, and Roswell (App. A), but mean monthly temperatures never fall below 0 °C. In order to keep temperatures within the ideal range, one could, for example, either decrease mean monthly temperature by 5 °C for Yuma, Phoenix, or Tucson or raise mean monthly temperature by 5 °C for El Paso, Albu-

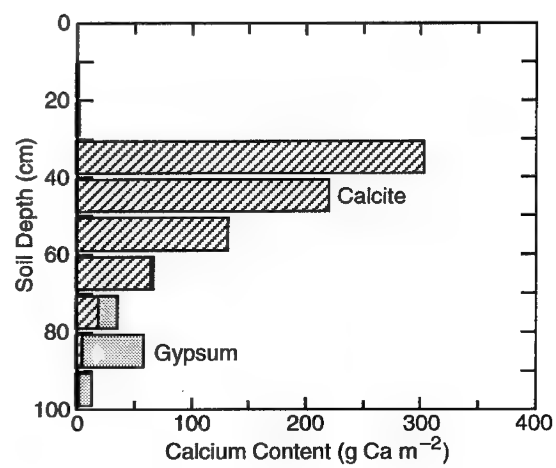

Figure 8. Accumulation of calcite and gypsum in a 1000-year simulation for the Tucson site (data in Table 2).

querque, Clayton, or Roswell, but not vice-versa (App. A). The temperature change is specified in a screen prompt under "Altered Climate."

Rain patterns can be altered by simply changing the data in *Detrain* for the deterministic model or by changing the frequency distributions for the stochastic model. To alter the rain pattern in the stochastic model requires explicitly changing "seasonal" patterns. In the current model, the interarrival days (variable "Inter," App. A) for Tucson in the winter is given by

0, 1, 2, 3, 4, 7, 10, 15, 25, 40, 57.

Changing these days to:

0, 1, 2, 3, 4, 5, 6, 8, 10, 12, 15

while holding the corresponding probabilities in "Freq" constant has the result of decreasing the interarrival time between rain events, and thereby increasing the number of winter rainfall events. Similarly, changing the rainfall amounts (variable "R") for Tucson-winter from

0.00, 0.25, 0.50, 0.75, 1.00, 1.25, 1.50, 1.75, 2.00, 3.00, 7.52

to

0.00, 0.25, 0.50, 0.75, 1.00, 1.25, 1.50, 2.00, 3.00, 5.00, 9.50

while holding the corresponding probabilities in "D" constant results in increasing the average rainfall amount/event. Together, these two changes in interarrival time and rainfall amounts increase the mean annual rainfall for Tucson from 28.6 cm (Tables 2 and 3) to 43.4 cm, a 51.6 % change with all of the increase occurring in the winter months. Most of this change is caused by increasing the number of rainfall events from 44.1 $year^{-1}$ (Table 3) to 60.4 $year^{-1}$ (37.0% increase) and the remainder (14.6%) is caused by increased rain amounts/event. By trial-and-error, one can manipulate the stochastic model probability distributions to increase or decrease rain dates, rainfall amounts, or alter seasonal distributions. Rainmodule is included with CALGYP to facilitate these trial-and-error calculations.

Provided temperatures remain within the range of model parameterization (see previous discussion), the user can easily add new Southwestern desert sites to CALGYP. Adding new sites to CALGYP from outside the desert Southwest will require developing a new evapotranspiration algorithm. One needs to relate actual evapotranspiration to the soil–vegetative system of interest (e.g., deserts, forests, grasslands) (Fig. 5). Such an exercise is not trivial, but neither is it a major problem. In most cases, the type of information needed to develop these relationships is available in the literature. To extrapolate this model to sites where seasonal freezing is important will require changing how seasons are dealt with. For example, winter might accumulate water as snow, allowing for a single leaching event with some fraction of winter snow in the spring. Because CALGYP is structured by seasons, incorporating frozen seasons should not be a major problem.

Chemistry

In *Equil*, chemical equilibrium is maintained for the $CaSO_4^0$ ion-pair and the precipitation-dissolution of calcite and gypsum. CALGYP uses a sequential approach to solving the chemical equilibrium equations. This approach is both simple and flexible. FREZCHEM, a chemical thermodynamic model for aqueous solutions at subzero temperatures, uses this approach and deals with ice formation and the precipitation-dissolution of 15 minerals (Marion and Grant 1994). To add new reactions means adding new chemical algorithms to the present sequence (See *Equil*). Depending on what the new reactions involve, the convergence criteria may need to be changed. At present the model iterates until the Ca^{2+} ion concentrations in successive iterations agree to within ± 1%. Other solution species or a suite of species could be used to test for mathematical convergence.

The upper limit of solution concentrations that CALGYP can handle is set by the range of validity of the Davies equation (eq 14), which is approximately 0.1 M (Davies 1962). Because of this limitation, adding a very soluble salt such as NaCl is not currently feasible. The solubility of NaCl at 25 °C is approximately 6.1 M (Marion and Grant 1994). To develop a model capable of working at high salt concentrations can be done using the Pitzer Equations (Plummer et al. 1988, Spencer et al. 1990, Pitzer 1991, Marion and Grant 1994).

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Appendix A. Program CALGYP.

4/18/94 10:09 Macintosh HD:MPW:CALGYP.f

```
      PROGRAM CALGYP

C  This is CALGYP.  The primary function is to calculate CaCO3 and
C  CaSO4 deposition in soils.  This program will run using current
C  climatic drivers for El Paso, Albuquerque, Clayton, Roswell, Yuma,
C  Phoenix, and Tucson.  The model will also simulate altered climates.
C  You may specify a drier climate or a change in temperature directly;
C  see following input statements.  See technical report for
C  restrictions on temperature change.  To specify a wetter climate
C  requires manipulating the cumulative probability distributions for
C  rain dates or rainfall amounts for the appropriate season and site.
C  See accompanying technical report for suggestions on how this might
C  be done.

      REAL Midmc, Mc, Ll,Isum, Leach, Leacca, Leachs
      REAL Mpotev(12),Midmoi(10),Moist(10),Lowerl(10)
      REAL ICO2(10),IBd(10),IHs(10),Loss(10)
      REAL*4 Rnum,rand
      INTEGER Site,Climat,Hori,Year,Years,Pint,S,Sumfre,Days(12),Seed
      DIMENSION Thick(10), Bd(10), Bar01(10), Bar15(10),
     X      Ca(10), CO2Mul(12), SO4(10), Temp(7,12),
     X      Upperl(10), Whc(10),Tis(12), Dpotev(12),
     X      Availw(10), Poresp(10)
      CHARACTER*50 Title
      DOUBLE PRECISION SO4s,CaCO3,CaSO4,Cas,Ka,Hs
      DOUBLE PRECISION Moisco,Horizo,Gain

      COMMON / Precipitation / Rain(200), Rainda(200),Sumfre,Site,
     x      Delrai,Numb,Rnum,Inter(7,3,11),Freq(7,3,11),R(7,3,11),
     x      D(7,3,11)
      COMMON / Chemistry / SO4s(10),CaCO3(10),CaSO4(10),Cas(10),Dhc,
     x      CO2(10),Hs(10),Ka(6),Moisco(10),Horizo(10),Gain(10)

      OPEN (UNIT = 2, FILE = "CaData")

C  Read in the program data

      PRINT*, 'Select Site:'
      PRINT*, '   1 = El Paso, TX (21.6cm)'
      PRINT*, '   2 = Albuq., NM (21.1cm)'
      PRINT*, '   3 = Clayton, NM (37.8cm)'
      PRINT*, '   4 = Roswell, NM (31.6cm)'
      PRINT*, '   5 = Yuma, AZ (8.5cm)'
      PRINT*, '   6 = Phoenix, AZ (18.9cm)'
      PRINT*, '   7 = Tucson, AZ (28.4cm)'
      READ*, Site

      Deltem = 0.0
      Delrai = 0.0

      PRINT*, 'Climate Option? Current Climate = 1, Altered Climate = 2'
      READ*, Climat
      IF (Climat .eq. 2) THEN
            PRINT*,'Enter Delta Temperature=(°C,default=0.0,no change)'
            READ*, Deltem
            PRINT*, 'Enter Fractional Change in Rainfall Amount during'
            PRINT*, '       Drier Climate = (default = 0.0, no change)'
            READ*, Delrai
      END IF

C  Days/Month

      DATA Days /31,28,31,30,31,30,31,31,30,31,30,31/
```

```
C  Monthly Temperatures

      DATA((Temp(I,J),J=1,12),I=1,7) /
     x      7.1,9.6,13.1,17.6,22.3,27.1,27.8,26.8,23.8,18.1,11.3,7.3,    El Paso
     x      1.4,4.3,8.1,12.7,17.7,23.1,25.2,24.1,20.3,13.8,6.6,1.8,      Albuq
     x      0.6,2.4,5.2,10.7,15.6,20.9,23.3,22.4,18.4,12.8,5.6,2.1,      Clayton
     x      4.2,6.6,10.6,15.3,20.1,24.8,26.2,25.4,21.6,15.4,8.8,4.5,     Roswell
     x      12.8,15.1,17.8,21.4,25.2,29.8,33.4,32.9,29.8,23.5,17.2,13.3,Yuma
     x      11.1,13.2,15.9,20.0,24.6,29.7,32.8,31.8,28.8,22.2,15.6,11.6,Phoenix
     x      10.2,11.8,14.3,18.1,22.6,27.8,30.0,28.9,26.7,20.8,14.6,10.8/Tucson

C Read in Stochastic Rain Model Parameters

      DATA (((D(I,J,K),K=1,11),J=1,2),I=1,7) /
     x      .000,.571,.745,.827,.837,.888,.918,.939,.959,.990,1.000,     EP,WINT
     x      .000,.526,.691,.773,.835,.866,.897,.938,.948,.979,1.000,     EP,SUM
     x      .000,.635,.832,.920,.964,.971,.986,.993,1.000,1.05,1.10,     AL,WINT
     x      .000,.577,.740,.827,.904,.952,.962,.981,.991,1.00,1.05,      AL,SUM
     x      .000,.586,.811,.928,.955,.982,.991,1.00,1.05,1.10,1.15,      CL,WINT
     x      .000,.371,.596,.728,.794,.860,.880,.933,.966,.986,1.000,     CL,SUM
     x      .000,.570,.756,.884,.907,.942,.965,1.00,1.05,1.10,1.15,      RS,WINT
     x      .000,.405,.628,.719,.769,.827,.868,.901,.975,.983,1.000,     RS,SUM
     x      .000,.512,.780,.865,.889,.938,.962,.986,1.00,1.05,1.10,      YU,WINT
     x      .000,.625,.875,1.000,1.05,1.10,1.15,1.20,1.25,1.30,1.35,     YU,SUM
     x      .000,.394,.567,.711,.817,.875,.923,.952,.971,.990,1.000,     PH,WINT
     x      .000,.600,.800,.933,1.000,1.1,1.2,1.3,1.4,1.5,1.6,           PH,SPR
     x      .000,.473,.661,.732,.803,.830,.875,.902,.947,.983,1.000,     TU,WINT
     x      .000,.550,.850,.950,1.000,2.0,3.0,4.0,5.0,6.0,7.0 /          TU,SPR

      DATA ((D(I,3,K),K=1,11),I=6,7) /
     x      .000,.642,.755,.793,.868,.925,.963,.982,1.000,1.5,2.0,       PH,SUM
     x      .000,.426,.539,.617,.730,.765,.843,.878,.913,.991,1.000 /    TU,SUM

      DATA (((R(I,J,K),K=1,11),J=1,2),I=1,7) /
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,2.00,3.00,3.07,         EP,WINT
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,2.00,4.00,5.59,         EP,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,2.00,2.64,3.00,5.00,         AL,WINT
     x      0.00,.25,.50,.75,1.00,1.25,1.50,2.00,3.00,4.45,10.0,         AL,SUM
     x      0.00,.25,.50,.75,1.00,1.25,2.00,4.83,5.00,10.0,15.0,         CL,WINT
     x      0.00,.25,.50,.75,1.00,1.50,2.00,3.00,4.00,5.00,5.36,         CL,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,5.00,10.0,15.0,         RS,WINT
     x      0.00,.25,.50,.75,1.00,1.50,2.00,3.00,5.00,7.00,10.72,        RS,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,3.00,4.45,10.0,16.0,         YU,WINT
     x      0.00,.25,.50,.58,1.00,1.25,1.50,1.75,2.00,3.00,3.07,         YU,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,2.00,3.00,5.03,         PH,WINT
     x      0.00,.25,.50,.75,.97,1.25,1.50,1.75,2.00,3.00,3.07,          PH,SPR
     x      0.00,.25,.50,.75,1.0,1.25,1.5,1.75,2.0,3.0,7.52,             TU,WINT
     x      0.00,.25,.50,.75,1.02,2.0,3.0,4.0,5.0,6.0,7.0 /              TU,SPR

      DATA ((R(I,3,K),K=1,11),I=6,7) /
     x      0.00,.25,.50,.75,1.00,1.50,2.00,3.50,4.22,5.00,10.0,         PH,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,2.00,3.00,3.23 /        TU,SUM

      DATA (((Freq(I,J,K),K=1,11),J=1,2),I=1,7) /
     x      0.00,.388,.449,.510,.531,.643,.765,.796,.888,.969,1.000,     EP,WINT
     x      0.00,.402,.454,.567,.680,.750,.853,.902,.923,.974,1.000,     EP,SUM
     x      0.00,.328,.447,.522,.589,.664,.768,.843,.910,.977,1.000,     AL,WINT
     x      0.00,.396,.481,.594,.679,.783,.840,.963,.982,.991,1.000,     AL,SUM
     x      0.00,.291,.409,.427,.472,.617,.762,.844,.944,.989,1.000,     CL,WINT
     x      0.00,.404,.530,.623,.716,.848,.901,.961,.987,.994,1.000,     CL,SUM
     x      0.00,.430,.488,.569,.616,.744,.825,.918,.988,1.000,1.05,     RS,WINT
     x      0.00,.380,.430,.521,.554,.703,.802,.918,.984,.992,1.000,     RS,SUM
```

```
     x      0.00,.316,.417,.430,.493,.582,.671,.785,.950,.988,1.000,     YU,WINT
     x      0.00,.111,.333,.777,1.000,1.05,1.1,1.2,1.3,1.4,1.5,          YU,SUM
     x      0.00,.476,.515,.583,.641,.719,.787,.865,.923,.972,1.000,     PH,WINT
     x      0.00,.250,.313,.438,.501,.564,.689,.814,.939,1.00,1.05,      PH,SPR
     x      0.00,.447,.552,.596,.631,.745,.815,.885,.955,.973,1.000,     TU,WINT
     x      0.00,.222,.278,.334,.390,.501,.612,.779,.890,.946,1.000 /    TU,SPR

      DATA ((Freq(I,3,K),K=1,11),I=6,7) /
     x      0.00,.212,.347,.482,.559,.713,.790,.886,.963,1.00,1.05,      PH,SUM
     x      0.00,.491,.640,.728,.781,.886,.965,.991,1.00,1.1,1.2 /       TU,SUM

      DATA (((Inter(I,J,K),K=1,11),J=1,2),I=1,7) /
     x      0,1,2,3,4,7,10,15,20,30,57,                                  EP,WINT
     x      0,1,2,3,4,7,10,15,20,30,66,                                  EP,SUM
     x      0,1,2,3,4,7,10,15,20,30,40,                                  AL,WINT
     x      0,1,2,3,4,7,10,15,20,30,32,                                  AL,SUM
     x      0,1,2,3,4,7,10,15,25,40,50,                                  CL,WINT
     x      0,1,2,3,4,7,10,13,15,20,21,                                  CL,SUM
     x      0,1,2,3,7,10,15,25,40,64,100,                                RS,WINT
     x      0,1,2,3,4,7,10,15,25,40,48,                                  RS,SUM
     x      0,1,2,3,4,7,10,15,40,70,111,                                 YU,WINT
     x      0,20,40,60,121,150,160,170,180,190,200,                      YU,SUM
     x      0,1,2,3,4,7,10,15,25,40,52,                                  PH,WINT
     x      0,1,5,10,15,25,40,50,60,77,100,                              PH,SPR
     x      0,1,2,3,4,7,10,15,25,40,57,                                  TU,WINT
     x      0,1,3,5,7,10,25,30,40,60,78 /                                TU,SPR

      DATA ((Inter(I,3,K),K=1,11),I=6,7) /
     x      0,1,2,3,4,7,10,15,20,24,50,                                  PH,SUM
     x      0,1,2,3,4,7,10,15,17,40,50 /                                 TU,SUM

C  Basic Soil & Atm Parameters

C  Horizon Thickness (cm) and Bulk Density (g/cc)
      DATA Thick / 10*10.0 /
      DATA Bd / 10*1.44 /
C  Horizon Soil Water Conc. (%) at 0.1 Bar, 15 Bar, and Initial
      DATA Bar01 / 10*.122 /
      DATA Bar15 / 10*.039 /
      DATA Moist / 10*0.10 /
C  Horizon CaCO3 (%Ca) and Soluble Ca (%)
      DATA CaCO3 / 10*0.0 /
      DATA Ca / 10*6e-7 /
C  Horizon H Activity and CO2 Conc. (ATM)
      DATA Hs / 10*1e-8 /
      DATA CO2 /3.79e-4,6.87e-4,9.76e-4,1.28e-3,1.60e-3,
     x      1.91e-3,2.14e-3,2.27e-3,2.41e-3,2.54e-3/
C  Monthly CO2 Multiplier
      DATA CO2Mul / 2*1.00,8*1.588,2*1.00 /
C  Horizon CaSO4 (%S) and Soluble SO4 (%S)
      DATA CaSO4 / 10*0.0 /
      DATA SO4 /10*1.0e-6/
C  Dust-Ca (g/cm2/day), Rain-Ca (mg/l), Rain-SO4-S (mg/l),
C  Dust-SO4-S (g/cm2/day)
      Dustca = 2.36e-7
      Precca = 0.00
      Precs = 0.00
      Dusts = 2.19e-8

C  Read In Basic Model Run Parameters

      PRINT*, 'Title?'
      READ(*,10) Title
```

```
10    FORMAT(A50)
      PRINT*, 'Number of Soil Horizons (Max=10)?'
      READ*, Hori
      PRINT*, 'Years to Simulate?'
      READ*, Years
      PRINT*, 'Print Interval?'
      READ*, Pint
      PRINT*, 'Deterministic (1) or Stochastic (2) Rainfall Model?'
      READ*, S
      IF (S .eq. 1)  GOTO 15
      PRINT*, 'Seed for Random Number Generator?'
      READ*, Seed
      Rnum = rand(Seed)

C  Convert Input to Program Units (% to g/cm2)

15    DO 20 I = 1, Hori
            Moisco(I)=Thick(I)*Bd(I)*Moist(I)
            Lowerl(I)=Thick(I)*Bd(I)*Bar15(I)
            Upperl(I)=Thick(I)*Bd(I)*Bar01(I)
            Whc(I)=Upperl(I)-Lowerl(I)
            Diff=Whc(I)*.546
            Midmoi(I)=Lowerl(I)+Diff
            CaCO3(I)=CaCO3(I)*Thick(I)*Bd(I)
            Ca(I)=Ca(I)*Thick(I)*Bd(I)
            CaSO4(I)=CaSO4(I)*Thick(I)*Bd(I)
            SO4(I)=SO4(I)*Thick(I)*Bd(I)
20    CONTINUE

C  Calculate Monthly Potential Evaporation using
C  Thornthwaite's Equation and Adjust to Pan Evaporation

      Isum = 0.0
      Totalt = 0.0
      DO 30 J = 1, 12
            Tis(J) = (Temp(Site,J)/5.0)**(1.514)
            Isum = Isum + Tis(J)
            Totalt = Totalt + Temp(Site,J)
30    CONTINUE
      Avert = Totalt/12.0
      Rat = (0.1278*EXP(.2802*(Avert+Deltem))+225.9)/
     x      (0.1278*EXP(.2802*Avert)+225.9)
      A=(6.75e-7*(Isum**3.0))-(7.71e-5*(Isum**2.0))+
     x      (1.792e-2*Isum+.49239)
      DO 40 J = 1, 12
            Mpotev(J) = 1.6*((10.0*Temp(Site,J)/Isum)**A)*Days(J)/30.0
            Dpotev(J) = Mpotev(J) / Days(J)
            IF (J .le. 7) THEN
                  Y = 17.07*EXP(-.1309*Temp(Site,J))+1.91
            ELSE
                  Y = 13.67*EXP(-.1300*Temp(Site,J))+1.35
            END IF
            Dpotev(J) = Y*Dpotev(J)*Rat
            Mpotev(J) = Y*Mpotev(J)*Rat
            Temp(Site,J) = Temp(Site,J)+Deltem
40    CONTINUE

C  Print the Initial State of the System

      WRITE (2,42) Title
42    FORMAT (A50)
      WRITE (2,*) 'SITE =', Site
      IF (S .eq. 1) WRITE (2,*) 'Deterministic Rainfall Model'
```

```
      IF (S .eq. 2) WRITE (2,*) 'Stochastic Rainfall Model with Seed =',
     x      Seed
      WRITE (2,*)
      WRITE (2,*) '    CLIMATIC SUMMARY'
      WRITE (2,*) '          Month    Temp(C)  Pot.Evap.(g/cm2)'
      DO 50 I = 1, 12
            WRITE (2,45) I, Temp(Site,I), Mpotev(I)
45          FORMAT(10X,I2,6X,F4.1,8X,F5.2)
50    CONTINUE
      WRITE (2,*)
      WRITE (2,*) 'INITIAL SOIL PROFILE'
      WRITE (2,*) 'Hori Thick  BD      CO2         H        CaCO3
     x       Ca         CaSO4        SO4'
      WRITE (2,*) '      cm   g/cm3    atm                 gCa/cm2
     x    gCa/cm2     gS/cm2     gS/cm2'
      DO 60 I = 1, Hori
            WRITE (2,55) I, Thick(I), Bd(I), CO2(I), Hs(I), CaCO3(I),
     x            Ca(I), CaSO4(I), SO4(I)
55          FORMAT(1X,I2,F6.1,F6.2,6E11.3)
60    CONTINUE
      WRITE (2,*)
      WRITE (2,*) 'ATMOSPHERIC CHEMICAL CONDITIONS'
      Dca=Dustca*365.0
      Ds=Dusts*365.0
      WRITE (2,*) 'Dustca(gCa/cm2/yr)  Precca(mgCa/l)
     x  Dusts(gS/cm2/yr)  Precs(mgS/l)'
      WRITE (2,65) Dca, Precca, Ds, Precs
65    FORMAT (2X,E12.4,F12.2,11X,E12.4,F12.2)

C  Initialize the Program Parameters

      DO 70 I = 1, Hori
            Ca(I) = Ca(I)/40.08
            SO4(I) = SO4(I)/32.064
            ICO2(I) = CO2(I)
            IBd(I) = Bd(I)
            IHs(I) = Hs(I)
70    CONTINUE
      Year = 1
      Leach = 0
      Leacca = 0
      Acumca = 0
      Leachs = 0
      Accums = 0
      Torain = 0
      Toevap = 0
      Inte = 0
      Cement = 0
100   Rdays = 0
      Tdays = Days(1)
      J=1
      I=1
      CALL CONSTANTS(Ka, Temp(Site,1),Dhc)
      Tevap = 0
      Train = 0
      Day = 0
      Midmc = 0
      Mc = 0
      Ll = 0
      Ul = 0
      DO 110 K = 1, Hori
            Ll = Ll + Lowerl(K)
            Ul = Ul + Upperl(K)
```

```
            Midmc = Midmc + Midmoi(K)
110    CONTINUE

C  Calculate Seasonal Precipitation Patterns

       IF (S .eq. 1) THEN
             CALL Detrain
       ELSE
             CALL Raindate
             CALL Rainfall
       END IF

       DO 120 Ijk = 1, Sumfre
             Train = Train + Rain(Ijk)
120    CONTINUE

C  Update Day, Month, and Equilibrium Constants

125    Day = Day + 1
       Acumca = Acumca + Dustca
       Accums = Accums + Dusts
       IF (Day .gt. Tdays) THEN
             I = I + 1
             DO 130 K = 1, Hori
                   CO2(K)  = ICO2(K)*CO2Mul(I)
130          CONTINUE
             Tdays = Tdays + Days(I)
             CALL CONSTANTS(Ka, Temp(Site,I),Dhc)
       END IF

C  Calculate the Loss of Soil Moisture from the
C  Profile During the Drying Cycle

       Do 140 K = 1, Hori
             Mc = Mc + Moisco(K)
140    CONTINUE
       IF (Mc .gt. Midmc) THEN
             Devap = Dpotev(I)
             Mc = 0.0
       ELSE
             Soilfa = (Mc-Ll)/(Midmc-Ll)
             Mc = 0.0
             Devap = Dpotev(I)*Soilfa
       END IF
       Tevap = Tevap + Devap
       DO 150 K = 1, Hori
             Availw(K)=Moisco(K)-Lowerl(K)
             IF (Availw(K) .gt. Devap) THEN
                   Loss(K) = Devap
                   Moisco(K) = Moisco(K)-Loss(K)
                   Devap = 0.0
                   GOTO 160
             ELSE
                   Loss(K) = Availw(K)
                   Moisco(K) = Lowerl(K)
                   Devap = Devap-Loss(K)
             END IF
150    CONTINUE
160    IF (Devap .gt. 0) Tevap = Tevap-Devap
       IF ((Rdays .eq. 1) .and. (Day .lt. 365)) GOTO 125
170    IF (Day .eq. 365) GOTO 180
       IF (Day .lt. Rainda(J)) GOTO 125
       IF (Rain(J) .eq. 0) THEN
```

```
          J = J + 1
          GOTO 125
      END IF

C  Calculate the Precipitation of CaCO3 & CaSO4 During the Drying Cycle

180   DO 190 K = 1, Hori
          Horizo(K) = 0.0
          Gain (K) = 0.0
          Cas(K) = Ca(K)*1000.0/Moisco(K)
          SO4s(K) = SO4(K)*1000.0/Moisco(K)
          CALL EQUIL(K)
          Ca(K) = Cas(K)*Moisco(K)/1000.0
          SO4(K) = SO4s(K)*Moisco(K)/1000.0
190   CONTINUE
      IF ((Rainda(J) .ne. 365) .and. (Day .eq. 365)) GOTO 300

C  Calculate the Gain of Water During the Wetting Cycle

200   Prec = Rain(J)
      DO 210 K = 1, Hori
          Availw(K) = Upperl(K) - Moisco(K)
          IF (Availw(K) .gt. Rain(J)) THEN
              Moisco(K) = Moisco(K) + Rain(J)
              Gain(K) = Rain(J)
              Rain(J) = 0.0
              GOTO 220
          ELSE
              Gain(K) = Availw(K)
              Moisco(K) = Moisco(K) + Gain(K)
              Rain(J) = Rain(J) - Gain(K)
          END IF
210   CONTINUE
220   IF ((Rain(J) .gt. 0) .and. (Cement .eq. 0)) Leach = Leach+Rain(J)

C  Calculate the Rain that Enters Each Horizon

      Horizo(1) = Prec
      DO 230 K = 2, Hori
          Horizo(K) = Horizo(K-1)-Gain(K-1)
230   CONTINUE

C  Calculate the Atmospheric Solution Chemistry

      Acumca = Acumca + Precca*Prec/1.0e6
      Caa = Acumca/40.08
      Acumca = 0.0
      Accums = Accums+Precs*Prec/1.0e6
      SO4a = Accums/32.064
      Accums = 0.0

C  Mix Horizon Solutions and Reestablish Equilibrium

      DO 240 K = 1, Hori
          Cas(K)=(Caa+Ca(K))*1000/(Horizo(K)+Moisco(K)-Gain(K))
          SO4s(K)=(SO4a+SO4(K))*1000/(Horizo(K)+Moisco(K)-Gain(K))
          CALL EQUIL(K)
          Caa = Cas(K)*(Horizo(K)-Gain(K))/1000
          Ca(K) = Cas(K)*Moisco(K)/1000
          SO4a = SO4s(K)*(Horizo(K)-Gain(K))/1000
          SO4(K) = SO4s(K)*Moisco(K)/1000
240   CONTINUE
      IF ((Rain(J).gt.0).and.(Cement.eq.0)) Leacca=Leacca+Cas(K-1)*
```

```
     x      Rain(J)*40.08/1000
      IF ((Rain(J).gt.0).and.(Cement.eq.0)) Leachs=Leachs+SO4s(K-1)*
     x      Rain(J)*32.064/1000
      IF (Cement.eq.1) CaCO3(K-1)=CaCO3(K-1)+Cas(K-1)*Rain(J)*40.08/1000
      IF (Cement.eq.1) CaSO4(K-1)=CaSO4(K-1)+SO4s(K-1)*
     x      Rain(J)*32.064/1000
      Rain(J) = 0.0

C  Update Rainday

      DO 250 K = 1, Hori
            Gain(K) = 0.0
            Loss(K) = 0.0
250   CONTINUE
      J = J + 1
      IF (J .gt. Sumfre) THEN
            Rdays = 1
            J = J - 1
            IF (Rainda(J) .eq. 365) GOTO 300
      ELSE
            IF (Rain(J) .eq. 0) J=J+1
      END IF
      GOTO 125

C  Update Soil Physical Parameters

300   DO 310 K = 1, Hori
            Bd(K)=IBd(K)+CaCO3(K)*100.09/(Thick(K)*40.08)+CaSO4(K)*
     x            172.17/(Thick(K)*32.064)
            IF (Bd(K) .gt. 2) THEN
                  Hori = K - 1
                  Cement = 1
                  GOTO 320
            ELSE
                  Poresp(K) = (1.0-Bd(K)/2.65)
                  IF (Poresp(K)*Thick(K) .gt. Whc(K)) GOTO 305
                  Upperl(K)=Upperl(K)-(Whc(K)-Poresp(K)*
     x                  Thick(K))
                  Whc(K) = Upperl(K)-Lowerl(K)
                  Diff = Whc(K)*.546
                  Midmoi(K) = Lowerl(K) + Diff
305         END IF
310   CONTINUE

C  Print Results

320   Inte = Inte + 1
      Torain = Torain + Train
      Toevap = Toevap + Tevap
      IF (Inte .ne. Pint) GOTO 350
330   WRITE (2,*)
      WRITE (2,*) '-----------------------------------------------------
     x-------------------------------'
      WRITE (2,*)
      WRITE (2,*) 'YEAR =', Year
      WRITE (2,*)
      WRITE (2,335) (CaCO3(J),J=1,Hori)
335   FORMAT('CACO3(gCa/cm2) =',5E12.5)
      WRITE (2,*)
      WRITE (2,336) (CaSO4(J),J=1,Hori)
336   FORMAT('CASO4(gS/cm2) =',5E12.5)
      WRITE (2,*)
      WRITE (2,337) (Bd(J),J=1,Hori)
```

```
337   FORMAT('Bulk Density(g/cm3) =',5F8.4)
      WRITE (2,*)
      WRITE (2,345) Leach, Leacca, Leachs
345   FORMAT('Leach(cm) =',E11.4,2X,'Leacca(gCa/cm2) =',E11.5,2X,
     x       'Leachs(gS/cm2) =',E11.5)
      WRITE (2,*)
      WRITE(2,347) Train,Tevap
347   FORMAT('Annual Rain(cm) =',F7.3,5X,'Annual Evap(cm) =',F7.3)
      Inte = 0

C  Update Year and Print Final Profile Concentrations

350   Year = Year + 1
      IF (Year .le. Years) GOTO 100
      WRITE (2,*)
      WRITE (2,*) '-------------------------------------------------
     x------------------------------'
      WRITE (2,*)
      WRITE (2,*) 'FINAL SOIL PROFILE CONCENTRATIONS'
      WRITE (2,*) ' See last year above for other final soil properties'
      WRITE (2,*)
360   WRITE (2,365)
365   FORMAT('Hori',2X,'Moisco(g/cm2)',3X,'H activity',5X,'Ca(gCa/cm2)
     x',4X,'SO4(gS/cm2)')
      DO 370 I = 1, Hori
            Ca(I) = Ca(I)*40.08
            SO4(I) = SO4(I)*32.064
            WRITE (2,367) I,Moisco(I), Hs(I), Ca(I), SO4(I)
367         FORMAT(1X,I2,4X,E12.5,3X,E12.5,3X,E12.5,3X,E12.5)
370   CONTINUE
      WRITE (2,*)
      WRITE(2,375) Torain, Toevap
375   FORMAT('Torain(cm) =',1X,E15.6,5X,'Toevap(cm) =',1X,E15.6)
      WRITE (2,*)
      WRITE(2,376) Acumca,Accums
376   FORMAT('Residual Dust Ca(gCa/cm2) =',E11.4,5X,'Residual Dust SO4
     x(gS/cm2) =',E11.4)
      END
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
      SUBROUTINE Detrain

C  Subroutine for Deterministic Rain Model.  The Dimension statement,
C  DATA, and Sumfre must be Changed for each Specific Site.

      DIMENSION Raindy(45), Raina(45)
      INTEGER Sumfre, Site
      COMMON / Precipitation / Rain(200), Rainda(200), Sumfre, Site,
     x       Delrai, Numb, Rnum, Inter(7,3,11), Freq(7,3,11), R(7,3,11),
     x       D(7,3,11)
      DATA Raindy / 9,10,11,19,21,29,31,39,44,45,
     x       46,47,49,52,66,69,70,78,85,86,
     x       120,172,180,181,187,193,200,204,206,208,
     x       210,214,225,226,235,236,248,250,267,
     x       268,269,288,289,340,346 /
      DATA Raina / .03,.05,.10,.61,.61,.15,.05,2.18,2.11,.99,
     x       1.14,.05,.05,.05,.10,.48,.36,.38,1.47,.30,
     x       .20,.20,.03,.36,.25,1.60,.84,.03,.38,.10,
     x       .18,.08,1.75,1.09,.18,1.47,.74,2.74,.99,
     x       1.98,.91,.05,.51,.10,.38 /

      Sumfre = 45
```

```
      DO 440 Ijk = 1, Sumfre
            Rainda(Ijk) = Raindy(Ijk)
            Rain(Ijk) = Raina(Ijk)
440   CONTINUE
      RNumb = Delrai*(Sumfre)
      Numb = NINT(RNumb)
      DO 450 I = 1, Numb
            RI = I
            RNumb = Numb
            Sum = Sumfre
            Elim = RI*Sum/RNumb
            Elim = INT(Elim)
            Rain(Elim) = 0
450   CONTINUE
      RETURN
      END
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
      SUBROUTINE Raindate

C  Calculate rain dates using a stochastic model
C  Present model developed for seven southwestern sites
C  Frequency distributions need to be changed for other sites

      REAL Newday(100), S(10), Intday
      REAL*4 Rnum, rand
      INTEGER Site, Season, X, Y, Sumfre
      COMMON / Precipitation / Rain(200),Rainda(200),Sumfre,Site,
     x      Delrai, Numb,Rnum,Inter(7,3,11),Freq(7,3,11),R(7,3,11),
     x      D(7,3,11)

C  Calculate Raindates

      J = 1
      Day = 0
485   CALL SEASONS(Site,Season,Day,Numb,Newj)
      DO 490 I = 1, 10
            S(I)=(Inter(Site,Season,I+1)-Inter(Site,Season,I))/
     x            (Freq(Site,Season,I+1)-Freq(Site,Season,I))
490   CONTINUE
      Rnum = rand(0)
      DO 500 I = 2, 11
            IF (Rnum .lt. Freq(Site,Season,I)) GOTO 510
500   CONTINUE
510   Intday=Inter(Site,Season,I-1)+S(I-1)*(Rnum-Freq(Site,Season,I-1))
     x+1.000
      Day = Day+Intday
      IF (Day .gt. 365) GOTO 515
      Rainda(J) = Day
      J = J+1
      GOTO 485

515   J = J-1

      IF (Newj .eq. 0) GOTO 555

C  Add new raindates to reproduce long-term mean (if necessary)
C  and sort dates numerically

      DO 520 I = 1, Newj
            Rnum = rand(0)
            Newday(I) = Rnum*364+1.000
```

```
520   CONTINUE
      J = J+Newj
      Ja = J+1-Newj
      I = 1
      DO 530 K = Ja, J
            Rainda(K) = Newday(I)
            I = I+1
530   CONTINUE
      Jb = J-1
      DO 550 X = 1, J
            DO 540 Y = 1, Jb
                  IF (Rainda(Y) .le. Rainda(Y+1)) GOTO 540
                  Tempor = Rainda(Y)
                  Rainda(Y) = Rainda(Y+1)
                  Rainda(Y+1) = Tempor
540         CONTINUE
550   CONTINUE

C  Eliminate Duplicate Raindates

555   Dup = 0
      I = 2
560   N = I+1
      IF (INT(Rainda(I)) .eq. INT(Rainda(I-1))) THEN
            Dup = Dup+1
            IF (N .gt. J) GOTO 575
            DO 570 K = N, J
                  Rainda(K-1) = Rainda(K)
570         CONTINUE

575         J = J-1
      END IF
      I = I+1
      IF (I .le. J) GOTO 560
      IF (Dup .gt. 0) GOTO 555

C  Return to CALGYP with New Raindates

      Sumfre = J
      DO 580 I = 1, Sumfre
            Rainda(I) = INT(Rainda(I))
580   CONTINUE
      RETURN
      END
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
      SUBROUTINE Rainfall

C  Calculate the storm rainfall amounts using a stochastic model
C  Present model developed for seven southwestern sites
C  Frequency distributions need to be changed for other sites.

      REAL S(10)
      REAL*4 Rnum, rand
      INTEGER Season, Site, Sumfre
      COMMON / Precipitation / Rain(200),Rainda(200),Sumfre,Site,
     x      Delrai,Numb,Rnum,Inter(7,3,11),Freq(7,3,11),R(7,3,11),
     x      D(7,3,11)

C  Calculate Rainfall Amounts

      J = Sumfre
```

```
      K = 1
600   CALL SEASONS(Site, Season, Rainda(K), Numb, Newj)
      DO 610 I = 1, 10
            S(I)=(R(Site,Season,I+1)-R(Site,Season,I))/
     x            (D(Site,Season,I+1)-D(Site,Season,I))
610   CONTINUE
      Rnum = rand(0)
      DO 620 I = 2, 11
            IF (Rnum .lt. D(Site,Season,I)) GOTO 630
620   CONTINUE
630   Rain(K) = R(Site,Season,I-1)+S(I-1)*(Rnum-D(Site,Season,I-1))
      K=K+1
      IF (K .le. J) GOTO 600

C  Set subset of rainfall amounts to zero to reproduce long-term
C  mean (if necessary) and to produce drier climates.

      RNumb = Numb + Delrai*(J-Numb)
      Numb = NINT(RNumb)
      Do 640 I=1, Numb
            RI = I
            RJ = J
            RNumb = Numb
            Elim = RI*RJ/RNumb
            Elim = INT(Elim)
            Rain(Elim)=0.0
640   CONTINUE

C  Return to CALGYP with New Rainfall Amounts

      RETURN
      END
C----------------------------------------------------------------------

C----------------------------------------------------------------------
      SUBROUTINE SEASONS(Site,Season,Day,Numb,Newj)

C This subroutine calculates the proper season for a given day and site

      INTEGER Site, Season

      IF (Site .eq. 1) THEN
            Numb=7
            Newj=0
            IF ((Day .lt. 152) .OR. (Day .gt. 304)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
      END IF

      IF (Site .eq. 2) THEN
            Newj = 7
            Numb=0
            IF ((Day .lt. 182) .OR. (Day .gt. 304)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
      END IF

      IF (Site .eq. 3) THEN
            Newj = 6
```

```
            Numb=0
            IF ((Day .lt. 121) .OR. (Day .gt. 273)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
      END IF

      IF (Site .eq. 4) THEN
            Numb=3
            Newj=0
            IF ((Day .lt. 121) .OR. (Day .gt. 304)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
      END IF

      IF (Site .eq. 5) THEN
            Numb=1
            Newj=0
            IF ((Day .lt. 91) .OR. (Day .gt. 212)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
      END IF

      IF (Site .eq. 6) THEN
            Numb=4
            Newj=0
            IF ((Day .lt. 91) .OR. (Day .gt. 273)) THEN
                  Season = 1
            ELSE
                  IF (Day .lt. 182) THEN
                        Season = 2
                  ELSE
                        Season = 3
                  END IF
            END IF
      END IF

      IF (Site .eq. 7) THEN
            Numb=9
            Newj=0
            IF ((Day .lt. 91) .OR. (Day .gt. 273)) THEN
                  Season = 1
            ELSE
                  IF (Day .lt. 182) THEN
                        Season = 2
                  ELSE
                        Season = 3
                  END IF
            END IF
      END IF

      RETURN
      END
C------------------------------------------------------------------------

C------------------------------------------------------------------------
      SUBROUTINE CONSTANTS(Ka,Temp,Dhc)
```

```
C  Calculate the Equilibrium Constants as Functions of Temperature

      DOUBLE PRECISION Ka(6)
      DIMENSION Pk(6)

      Pk(1) = 1.14+.0131*Temp
      Pk(2) = 6.54-.0071*Temp
      Pk(3) = 10.59-.0102*Temp
      Pk(4) = 7.95+.0125*Temp
      Pk(5) = 4.62+.0006*Temp
      Pk(6) = 2.23+.0019*Temp
      DO 480 K = 1, 6
            Ka(K) = EXP(-2.3026*Pk(K))
480   CONTINUE
      Dhc=0.4918+6.6098e-4*Temp+5.0231e-6*Temp**2
      RETURN
      END
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
      SUBROUTINE ION(Ionstr,Ac1,Ac2,Dhc)

C Calculate Uni- and Di-valent Activity Coefficients Using
C the Davies Equation

      REAL Ionstr

      Factor = SQRT(Ionstr)/(1.0+SQRT(Ionstr))-.3*Ionstr
      Ac1 = EXP(-2.3026*Dhc*Factor)
      Ac2 = EXP(-4*2.3026*Dhc*Factor)
      RETURN
      END
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
      SUBROUTINE Hact (CO2, Hs, SO4, Ac1, Ac2, Ka)

C  This is a subroutine to calculate the H activity for a
C  system in equilibrium with CaCO3 and CaSO4.

      DOUBLE PRECISION Ka(6),K1,K2,K3,F,Df,H,Dx,Hs,SO4
      DIMENSION Frac(8)
      H=Hs
      DATA Frac/.8,1.2,.5,1.5,.2,5.0,.1,10.0/
      I=1
      K1=2.0*Ka(4)/(Ka(3)*Ka(2)*Ka(1))
      K2=2.0*Ka(1)*Ka(2)*Ka(3)
      K3=Ka(1)*Ka(2)
375   F=K1*H**2/(CO2*Ac2)-K2*CO2/(H**2*Ac2)-K3*CO2/(H*Ac1)-2.0*SO4
      Df=2.0*K1*H/(CO2*Ac2)+K3*CO2/(H**2*Ac1)+2*K2*CO2/(H**3*Ac2)
      F=-1.0*F
      Dx=F/Df
      H=H+Dx
      Pcen=ABS(Dx/H)*100.0
      IF (Pcen .lt. 1) GOTO 380
      IF ((H .gt. 1.0e-5) .or. (H .lt. 1.0e-10)) THEN
            H=Hs*Frac(I)
            I=I+1
            IF (I .gt. 8) THEN
                  PRINT*,'The hydrogen subroutine will not converge'
                  GOTO 390
            END IF
      END IF
```

```
      GOTO 375
380   Hs=H
      RETURN
390   END
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
      SUBROUTINE EQUIL(K)

C  This is a subroutine to determine equilibrium concentrations of
C  solutes in saturated CaCO3 and CaSO4 solutions

      REAL I
      DOUBLE PRECISION A,B,C,X,Caion,SO4ion,Cas,SO4s,CaSO40,SysCa,
     xCaCO3,Pk4,Pk5,SysSO4,CaSO4,Pk6,Test,HCO3,CO3,Ka,Hs,Moisco,
     xHorizo,Gain
      COMMON / Chemistry / SO4s(10), CaCO3(10), CaSO4(10), Cas(10),Dhc,
     x      CO2(10), Hs(10), Ka(6), Moisco(10), Horizo(10), Gain(10)

C  Initiate Variables

      I = 3.0*Cas(K)
      Caion = Cas(K)
      Test = Caion
      IF ((SO4s(K) .EQ. 0.0) .AND. (CaSO4(K) .EQ. 0.0)) THEN
            SO4ion=0.0
            CaSO40=0.0
      END IF
460   CALL ION(I, Ac1, Ac2,Dhc)
      IF ((SO4s(K) .EQ. 0.0) .AND. (CaSO4(K) .EQ. 0.0)) GO TO 465

C  Calculate CaSO4 Ionpair

      Pk6 = Ka(6)/Ac2**2
      A = 1.0
      B = -1.0*(Cas(K)+SO4s(K)+Pk6)
      C = Cas(K)*SO4s(K)
      X = (-B-SQRT(B**2-4.0*A*C))/2.0*A
      Caion = Cas(K) - X
      SO4ion = SO4s(K) - X
      CaSO40 = X


C  Calculate CaCO3 Precipitation-Dissolution

465   IF (CaCO3(K) .gt. 0.0) CALL Hact(CO2(K),Hs(K),SO4ion,Ac1,Ac2,Ka)
      SysCa=Caion+CaCO3(K)*1000.0/(40.08*(Moisco(K)+Horizo(K)-
     x      Gain(K)))
      Pk4=(Hs(K)**2*Ka(4))/(Ac2*Ka(1)*Ka(2)*Ka(3)*CO2(K))
      X = SysCa-Pk4
      IF (X .lt. 0.0) X=0.0
      Caion = SysCa-X
      CaCO3(K)=(X)*40.08*(Moisco(K)+Horizo(K)-Gain(K))/1000.0
      IF ((SO4s(K) .EQ. 0.0) .AND. (CaSO4(K) .EQ. 0.0)) GO TO 467

C  Calculate CaSO4 Precipitation-Dissolution

      SysCa=Caion+CaSO4(K)*1000.0/(32.064*(Moisco(K)+Horizo(K)-
     x      Gain(K)))
      SysSO4=SO4ion+CaSO4(K)*1000.0/(32.064*(Moisco(K)+
     x      Horizo(K)-Gain(K)))
      Pk5 = Ka(5)/Ac2**2
      A = 1.0
```

```
      B = -1.0*(SysCa+SysSO4)
      C = SysCa*SysSO4-Pk5
      X = (-B-SQRT(B**2-4*A*C))/(2.0*A)
      IF (X .lt. 0.0) X = 0.0
      Caion = SysCa-X
      SO4ion = SysSO4-X
      CaSO4(K)=(X)*32.064*(Moisco(K)+Horizo(K)-Gain(K))/1000.0

C  Update Concentrations and Test for Convergence

467   Cas(K) = Caion+CaSO40
      SO4s(K) = SO4ion+CaSO40
      HCO3 = Ka(1)*Ka(2)*CO2(K)/(Hs(K)*Ac1)
      CO3=Ka(1)*Ka(2)*Ka(3)*CO2(K)/(Hs(K)**2*Ac2)
      I = .5*(4.0*(Caion+SO4ion+CO3)+HCO3)
      Diff = ABS((Test-Caion)/Caion)*100.0
      IF (Diff .gt. 1.0) THEN
            Test = Caion
            GOTO 460
      END IF

470   RETURN
      END
C-----------------------------------------------------------------------
```

Appendix B. Program RAINMODULE.

```
4/18/94 10:45                 Macintosh HD:MPW:RainMd.f

      PROGRAM RAINMODULE

C     This program calculates raindates and rainfall amounts using a
C     stochastic model for seven southwestern sites.

      INTEGER Site, Year, Sum, Sumfre, Totsum, Seed
      REAL *4 Rnum, rand
      CHARACTER*50 Title
      COMMON Rain(200), Rainda(200), Sumfre, Site, Delrai, Numb,Rnum,
     x      Inter(7,3,11), Freq(7,3,11), R(7,3,11), D(7,3,11)

C  Read in the program data

      PRINT*, 'Select Site:'
      PRINT*, '    1 = El Paso, TX (21.6cm)'
      PRINT*, '    2 = Albuq., NM (21.1cm)'
      PRINT*, '    3 = Clayton, NM (37.8cm)'
      PRINT*, '    4 = Roswell, NM (31.6cm)'
      PRINT*, '    5 = Yuma, AZ (8.5cm)'
      PRINT*, '    6 = Phoenix, AZ (18.9cm)'
      PRINT*, '    7 = Tucson, AZ (28.4cm)'
      READ*, Site

C  Read in basic model run parameters

      PRINT*, 'Title?'
      READ*, Title
      PRINT*, 'Fractional Change in Rain for Drier Climate.'
      PRINT*, '    Default = 0.00, no change.'
      READ*, Delrai
      PRINT*, 'Seed for Random Number Generator?'
      READ*, Seed
      Rnum = rand(Seed)
      PRINT*,'              Rain(cm)  Rain Events'

C Read in Stochastic Rain Model Parameters

      DATA (((D(I,J,K),K=1,11),J=1,2),I=1,7) /
     x      .000,.571,.745,.827,.837,.888,.918,.939,.959,.990,1.000,     EP,WINT
     x      .000,.526,.691,.773,.835,.866,.897,.938,.948,.979,1.000,     EP,SUM
     x      .000,.635,.832,.920,.964,.971,.986,.993,1.000,1.05,1.10,     AL,WINT
     x      .000,.577,.740,.827,.904,.952,.962,.981,.991,1.00,1.05,      AL,SUM
     x      .000,.586,.811,.928,.955,.982,.991,1.00,1.05,1.10,1.15,      CL,WINT
     x      .000,.371,.596,.728,.794,.860,.880,.933,.966,.986,1.000,     CL,SUM
     x      .000,.570,.756,.884,.907,.942,.965,1.00,1.05,1.10,1.15,      RS,WINT
     x      .000,.405,.628,.719,.769,.827,.868,.901,.975,.983,1.000,     RS,SUM
     x      .000,.512,.780,.865,.889,.938,.962,.986,1.00,1.05,1.10,      YU,WINT
     x      .000,.625,.875,1.000,1.05,1.10,1.15,1.20,1.25,1.30,1.35,     YU,SUM
     x      .000,.394,.567,.711,.817,.875,.923,.952,.971,.990,1.000,     PH,WINT
     x      .000,.600,.800,.933,1.000,1.1,1.2,1.3,1.4,1.5,1.6,           PH,SPR
     x      .000,.473,.661,.732,.803,.830,.875,.902,.947,.983,1.000,     TU,WINT
     x      .000,.550,.850,.950,1.000,2.0,3.0,4.0,5.0,6.0,7.0 /          TU,SPR

      DATA ((D(I,3,K),K=1,11),I=6,7) /
     x      .000,.642,.755,.793,.868,.925,.963,.982,1.000,1.5,2.0,       PH,SUM
     x      .000,.426,.539,.617,.730,.765,.843,.878,.913,.991,1.000 /    TU,SUM

      DATA (((R(I,J,K),K=1,11),J=1,2),I=1,7) /
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,2.00,3.00,3.07,         EP,WINT
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,2.00,4.00,5.59,         EP,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,2.00,2.64,3.00,5.00,         AL,WINT
     x      0.00,.25,.50,.75,1.00,1.25,1.50,2.00,3.00,4.45,10.0,         AL,SUM
     x      0.00,.25,.50,.75,1.00,1.25,2.00,4.83,5.00,10.0,15.0,         CL,WINT
```

```
     x      0.00,.25,.50,.75,1.00,1.50,2.00,3.00,4.00,5.00,5.36,          CL,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,5.00,10.0,15.0,          RS,WINT
     x      0.00,.25,.50,.75,1.00,1.50,2.00,3.00,5.00,7.00,10.72,         RS,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,3.00,4.45,10.0,16.0,          YU,WINT
     x      0.00,.25,.50,.58,1.00,1.25,1.50,1.75,2.00,3.00,3.07,          YU,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,2.00,3.00,5.03,          PH,WINT
     x      0.00,.25,.50,.75,.97,1.25,1.50,1.75,2.00,3.00,3.07,           PH,SPR
     x      0.00,.25,.50,.75,1.0,1.25,1.5,1.75,2.0,3.0,7.52,              TU,WINT
     x      0.00,.25,.50,.75,1.02,2.0,3.0,4.0,5.0,6.0,7.0 /               TU,SPR

      DATA ((R(I,3,K),K=1,11),I=6,7) /
     x      0.00,.25,.50,.75,1.00,1.50,2.00,3.50,4.22,5.00,10.0,          PH,SUM
     x      0.00,.25,.50,.75,1.00,1.25,1.50,1.75,2.00,3.00,3.23 /         TU,SUM

      DATA (((Freq(I,J,K),K=1,11),J=1,2),I=1,7) /
     x      0.00,.388,.449,.510,.531,.643,.765,.796,.888,.969,1.000,      EP,WINT
     x      0.00,.402,.454,.567,.680,.750,.853,.902,.923,.974,1.000,      EP,SUM
     x      0.00,.328,.447,.522,.589,.664,.768,.843,.910,.977,1.000,      AL,WINT
     x      0.00,.396,.481,.594,.679,.783,.840,.963,.982,.991,1.000,      AL,SUM
     x      0.00,.291,.409,.427,.472,.617,.762,.844,.944,.989,1.000,      CL,WINT
     x      0.00,.404,.530,.623,.716,.848,.901,.961,.987,.994,1.000,      CL,SUM
     x      0.00,.430,.488,.569,.616,.744,.825,.918,.988,1.000,1.05,      RS,WINT
     x      0.00,.380,.430,.521,.554,.703,.802,.918,.984,.992,1.000,      RS,SUM
     x      0.00,.316,.417,.430,.493,.582,.671,.785,.950,.988,1.000,      YU,WINT
     x      0.00,.111,.333,.777,1.000,1.05,1.1,1.2,1.3,1.4,1.5,           YU,SUM
     x      0.00,.476,.515,.583,.641,.719,.787,.865,.923,.972,1.000,      PH,WINT
     x      0.00,.250,.313,.438,.501,.564,.689,.814,.939,1.00,1.05,       PH,SPR
     x      0.00,.447,.552,.596,.631,.745,.815,.885,.955,.973,1.000,      TU,WINT
     x      0.00,.222,.278,.334,.390,.501,.612,.779,.890,.946,1.000 /     TU,SPR

      DATA ((Freq(I,3,K),K=1,11),I=6,7) /
     x      0.00,.212,.347,.482,.559,.713,.790,.886,.963,1.00,1.05,       PH,SUM
     x      0.00,.491,.640,.728,.781,.886,.965,.991,1.00,1.1,1.2 /        TU,SUM

      DATA (((Inter(I,J,K),K=1,11),J=1,2),I=1,7) /
     x      0,1,2,3,4,7,10,15,20,30,57,                                   EP,WINT
     x      0,1,2,3,4,7,10,15,20,30,66,                                   EP,SUM
     x      0,1,2,3,4,7,10,15,20,30,40,                                   AL,WINT
     x      0,1,2,3,4,7,10,15,20,30,32,                                   AL,SUM
     x      0,1,2,3,4,7,10,15,25,40,50,                                   CL,WINT
     x      0,1,2,3,4,7,10,13,15,20,21,                                   CL,SUM
     x      0,1,2,3,7,10,15,25,40,64,100,                                 RS,WINT
     x      0,1,2,3,4,7,10,15,25,40,48,                                   RS,SUM
     x      0,1,2,3,4,7,10,15,40,70,111,                                  YU,WINT
     x      0,20,40,60,121,150,160,170,180,190,200,                       YU,SUM
     x      0,1,2,3,4,7,10,15,25,40,52,                                   PH,WINT
     x      0,1,5,10,15,25,40,50,60,77,100,                               PH,SPR
     x      0,1,2,3,4,7,10,15,25,40,57,                                   TU,WINT
     x      0,1,3,5,7,10,25,30,40,60,78 /                                 TU,SPR

      DATA ((Inter(I,3,K),K=1,11),I=6,7) /
     x      0,1,2,3,4,7,10,15,20,24,50,                                   PH,SUM
     x      0,1,2,3,4,7,10,15,17,40,50 /                                  TU,SUM

      Inte = 1
      Torain = 0.0
      Totsum = 0.0
10    Year = 1
      Cenrai = 0.0
      Sum = 0
20    Train = 0.0

C Calculate Annual Rainfall Pattern
```

```
      CALL Raindate
      CALL Rainfall

      DO 30 Ijk = 1, Sumfre
            Train = Train + Rain(Ijk)
30    CONTINUE
      Sumfre = Sumfre - Numb
      Cenrai = Cenrai + Train
      Torain = Torain + Train
      Sum = Sum + Sumfre
      Totsum = Totsum + Sumfre

C  Update Annual Parameters

      Year = Year + 1
      IF (Year .LE. 100) GOTO 20

50    PRINT 60, Cenrai, Sum
60    FORMAT (1X,'100 yrs = ', F8.1, 3X, I6)
      Inte = Inte + 1
      IF (Inte .LE. 10) GOTO 10

70    PRINT 80, Torain, Totsum
80    FORMAT ('1000 yrs = ', F8.1, 3X, I6)
      PAUSE
      END

C---------------------------------------------------------------------------
C---------------------------------------------------------------------------

      SUBROUTINE Raindate

C  Calculate rain dates using a stochastic model
C  Present model developed for seven southwestern sites
C  Frequency distributions need to be changed for other sites

      REAL Newday(100), S(10), Intday
      REAL*4 Rnum, rand
      INTEGER Site, Season, X, Y, Sumfre
      COMMON Rain(200),Rainda(200),Sumfre,Site,
     x      Delrai, Numb,Rnum,Inter(7,3,11),Freq(7,3,11),R(7,3,11),
     x      D(7,3,11)

C  Calculate Raindates

      J = 1
      Day = 0
485   CALL SEASONS(Site,Season,Day,Numb,Newj)
      DO 490 I = 1, 10
            S(I)=(Inter(Site,Season,I+1)-Inter(Site,Season,I))/
     x             (Freq(Site,Season,I+1)-Freq(Site,Season,I))
490   CONTINUE
      Rnum = rand(0)
      DO 500 I = 2, 11
            IF (Rnum .lt. Freq(Site,Season,I)) GOTO 510
500   CONTINUE
510   Intday=Inter(Site,Season,I-1)+S(I-1)*(Rnum-Freq(Site,Season,I-1))
     x+1.000
      Day = Day+Intday
      IF (Day .gt. 365) GOTO 515
      Rainda(J) = Day
      J = J+1
```

```
      GOTO 485

515   J = J-1

      IF (Newj .eq. 0) GOTO 555

C  Add new raindates to reproduce long-term mean (if necessary)
C  and sort dates numerically

      DO 520 I = 1, Newj
            Rnum = rand(0)
            Newday(I) = Rnum*364+1.000
520   CONTINUE
      J = J+Newj
      Ja = J+1-Newj
      I = 1
      DO 530 K = Ja, J
            Rainda(K) = Newday(I)
            I = I+1
530   CONTINUE
      Jb = J-1
      DO 550 X = 1, J
            DO 540 Y = 1, Jb
                  IF (Rainda(Y) .le. Rainda(Y+1)) GOTO 540
                  Tempor = Rainda(Y)
                  Rainda(Y) = Rainda(Y+1)
                  Rainda(Y+1) = Tempor
540         CONTINUE
550   CONTINUE

C  Eliminate Duplicate Raindates

555   Dup = 0
      I = 2
560   N = I+1
      IF (INT(Rainda(I)) .eq. INT(Rainda(I-1))) THEN
            Dup = Dup+1
            IF (N .gt. J) GOTO 575
            DO 570 K = N, J
                  Rainda(K-1) = Rainda(K)
570         CONTINUE

575         J = J-1
      END IF
      I = I+1
      IF (I .le. J) GOTO 560
      IF (Dup .gt. 0) GOTO 555

C  Return to Rainmodule with New Raindates

      Sumfre = J
      DO 580 I = 1, Sumfre
            Rainda(I) = INT(Rainda(I))
580   CONTINUE
      RETURN
      END

C-------------------------------------------------------------------------
C-------------------------------------------------------------------------

      SUBROUTINE Rainfall

C  Calculate the storm rainfall amounts using a stochastic model
```

```
C  Present model developed for seven southwestern sites
C  Frequency distributions need to be changed for other sites.

      REAL S(10)
      REAL*4 Rnum, rand
      INTEGER Season, Site, Sumfre
      COMMON Rain(200),Rainda(200),Sumfre,Site,
     x      Delrai,Numb,Rnum,Inter(7,3,11),Freq(7,3,11),R(7,3,11),
     x      D(7,3,11)

C  Calculate Rainfall Amounts

      J = Sumfre
      K = 1
600   CALL SEASONS(Site, Season, Rainda(K), Numb, Newj)
      DO 610 I = 1, 10
            S(I)=(R(Site,Season,I+1)-R(Site,Season,I))/
     x            (D(Site,Season,I+1)-D(Site,Season,I))
610   CONTINUE
      Rnum = rand(0)
      DO 620 I = 2, 11
            IF (Rnum .lt. D(Site,Season,I)) GOTO 630
620   CONTINUE
630   Rain(K) = R(Site,Season,I-1)+S(I-1)*(Rnum-D(Site,Season,I-1))
      K=K+1
      IF (K .le. J) GOTO 600

C  Set subset of rainfall amounts to zero to reproduce long-term
C  mean (if necessary) and to produce drier climates.

      RNumb = Numb + Delrai*(J-Numb)
      Numb = NINT(RNumb)
      Do 640 I=1, Numb
            RI = I
            RJ = J
            RNumb = Numb
            Elim = RI*RJ/RNumb
            Elim = INT(Elim)
            Rain(Elim)=0.0
640   CONTINUE

C  Return to Rainmodule with New Rainfall Amounts

      RETURN
      END

C-----------------------------------------------------------------------
C-----------------------------------------------------------------------

      SUBROUTINE SEASONS(Site,Season,Day,Numb,Newj)

C This subroutine calculates the proper season for a given day and site

      INTEGER Site,Season

      IF (Site .eq. 1) THEN
            Numb=7
            Newj=0
            IF ((Day .lt. 152) .OR. (Day .gt. 304)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
```

```
      END IF

      IF (Site .eq. 2) THEN
            Newj = 7
            Numb=0
            IF ((Day .lt. 182) .OR. (Day .gt. 304)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
      END IF

      IF (Site .eq. 3) THEN
            Newj = 6
            Numb=0
            IF ((Day .lt. 121) .OR. (Day .gt. 273)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
      END IF

      IF (Site .eq. 4) THEN
            Numb=3
            Newj=0
            IF ((Day .lt. 121) .OR. (Day .gt. 304)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
      END IF

      IF (Site .eq. 5) THEN
            Numb=1
            Newj=0
            IF ((Day .lt. 91) .OR. (Day .gt. 212)) THEN
                  Season = 1
            ELSE
                  Season = 2
            END IF
      END IF

      IF (Site .eq. 6) THEN
            Numb=4
            Newj=0
            IF ((Day .lt. 91) .OR. (Day .gt. 273)) THEN
                  Season = 1
            ELSE
                  IF (Day .lt. 182) THEN
                        Season = 2
                  ELSE
                        Season = 3
                  END IF
            END IF
      END IF

      IF (Site .eq. 7) THEN
            Numb=9
            Newj=0
            IF ((Day .lt. 91) .OR. (Day .gt. 273)) THEN
                  Season = 1
            ELSE
                  IF (Day .lt. 182) THEN
```

```
                Season = 2
            ELSE
                Season = 3
            END IF
        END IF
    END IF
    RETURN
    END
```

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This report documents the CALGYP model which is designed to simulate calcite and gypsum precipitation–dissolution in soils. CALGYP is a process model that is easy to parameterize, and is designed for long-term simulations (> 1000 years). The CALGYP model has five components: soil parameterization, chemical thermodynamic relations, deterministic and stochastic rainfall models, an evapotranspiration model, and subroutines that calculate water, calcium, and sulfate fluxes through the soil. The stochastic rainfall model is based on probability distributions for interarrival times (days between rainfall events) and rainfall amounts and is designed to simulate the long-term mean annual rainfall and variability in annual rainfall for specific sites. The model is currently parameterized for seven climatic sites in the desert Southwest. However, climate (temperature and rainfall) can be altered and other minerals included, which makes the CALGYP model potentially applicable across a wider range of environmental conditions including freezing–thawing systems. A separate program, Rainmodule, is included to facilitate inclusion of new sites and to alter rainfall patterns for current sites. Instructions for utilization and a FORTRAN-77 source code listing are included with the report.

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